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Antiproliferative, antioxidant, computational and electrochemical studies of new azo-containing Schiff Base Ruthenium(II) complexes

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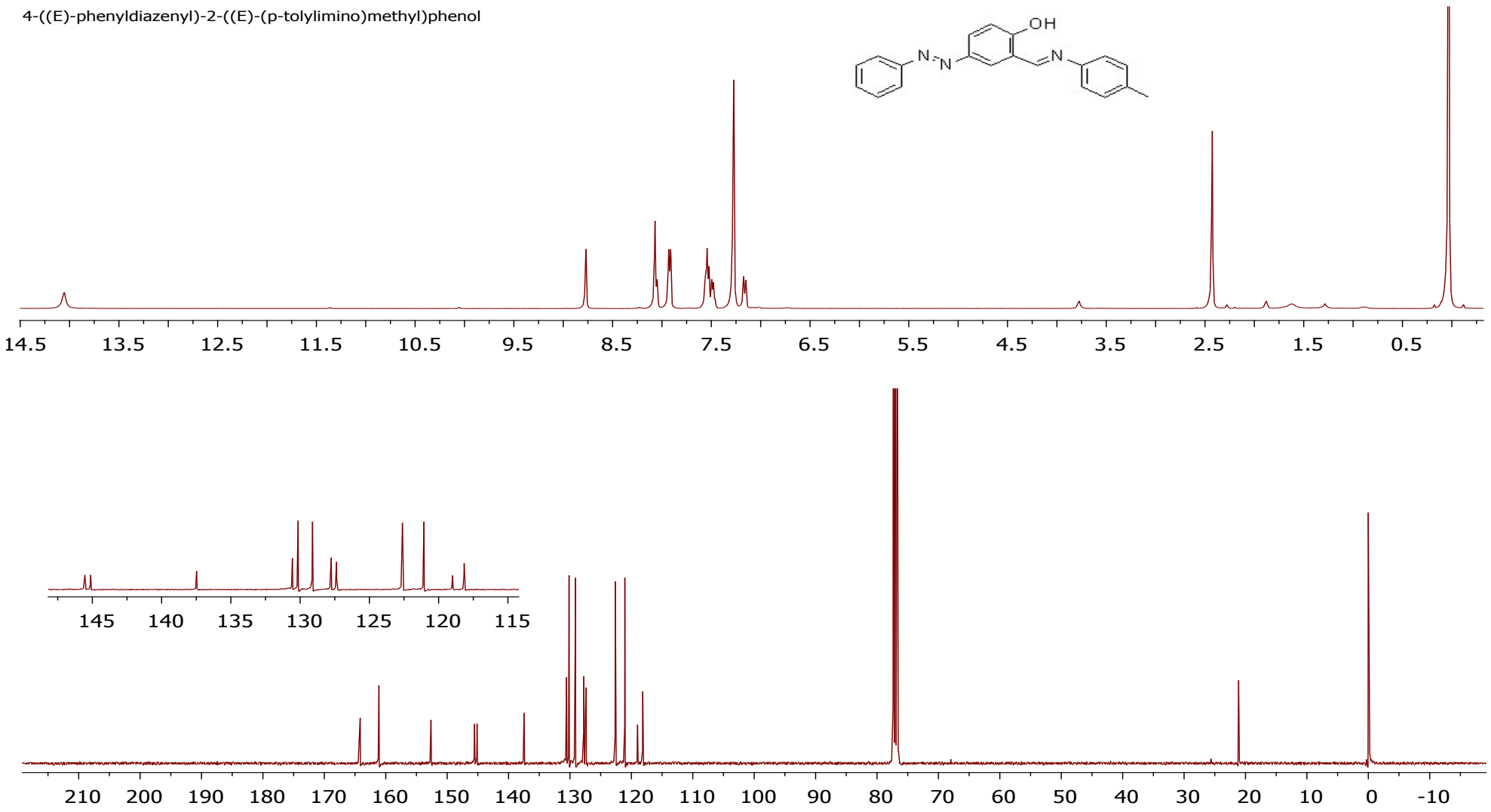

Fig. S1. ^{1}H and ^{13}C-NMR spectrum of **2**

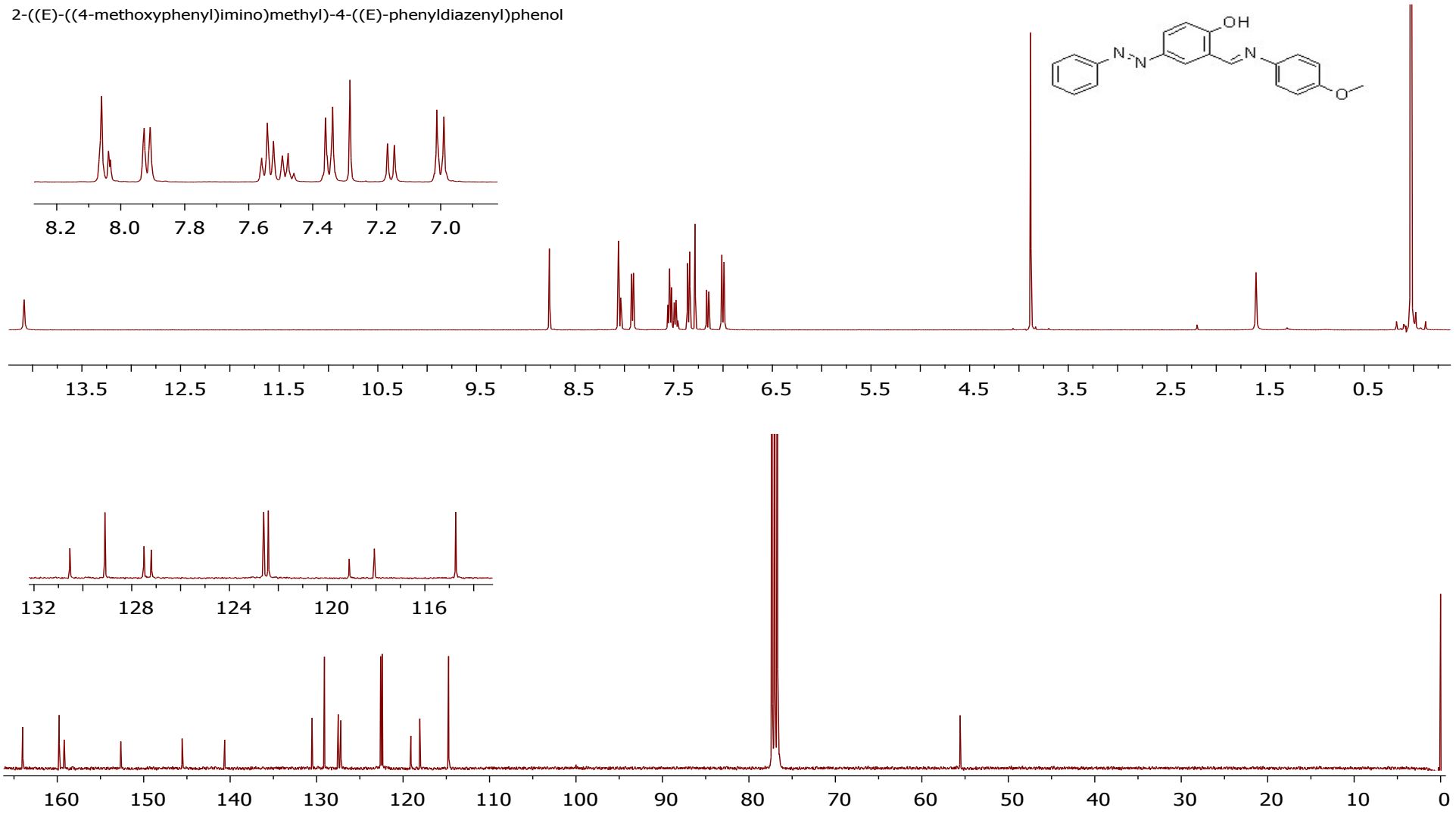

Fig. S2. ^{1}H and ^{13}C-NMR spectrum of **3**

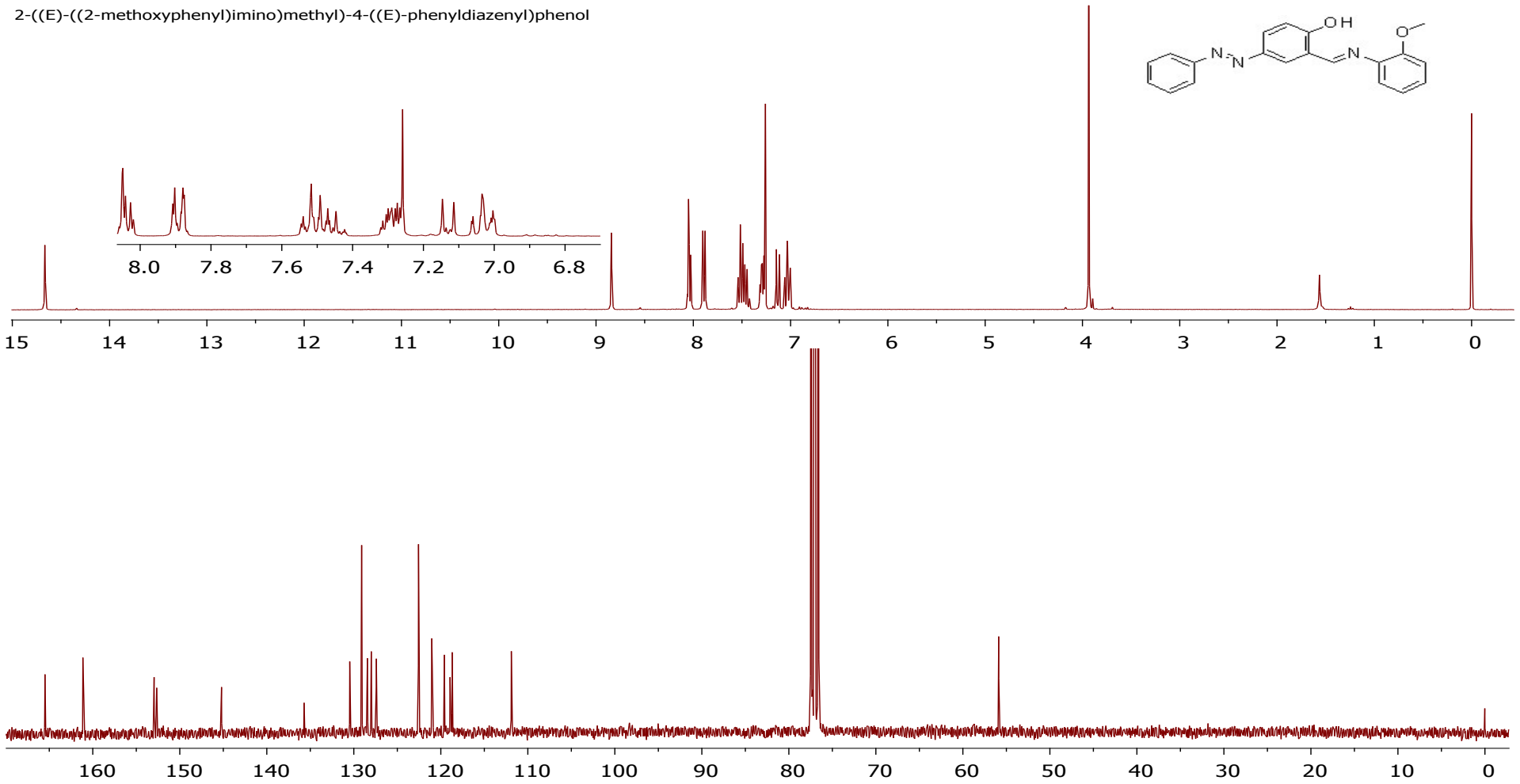

Fig. S3. ^{1}H and ^{13}C-NMR spectrum of **4**

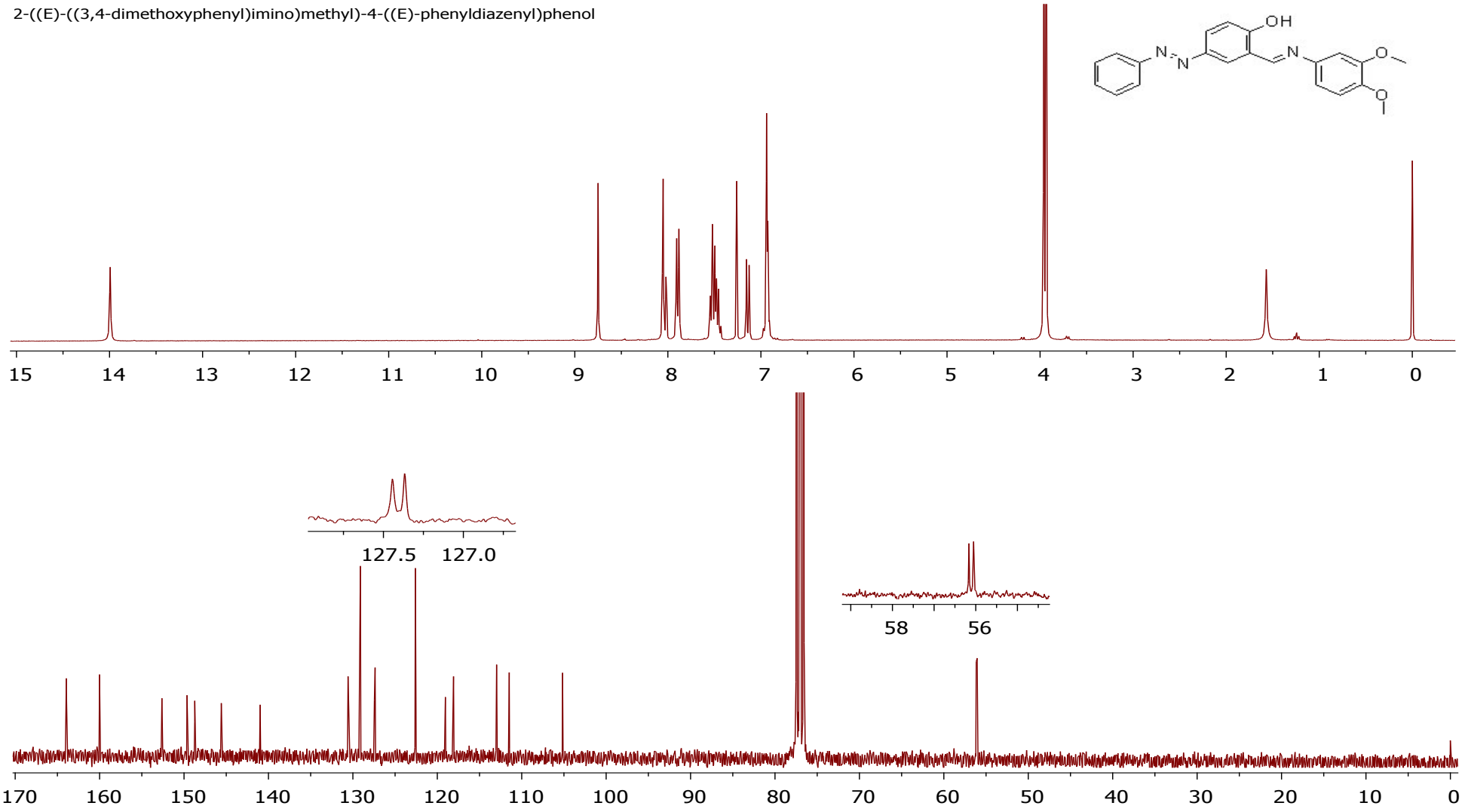

Fig. S4. ^{1}H and ^{13}C-NMR spectrum of **5**

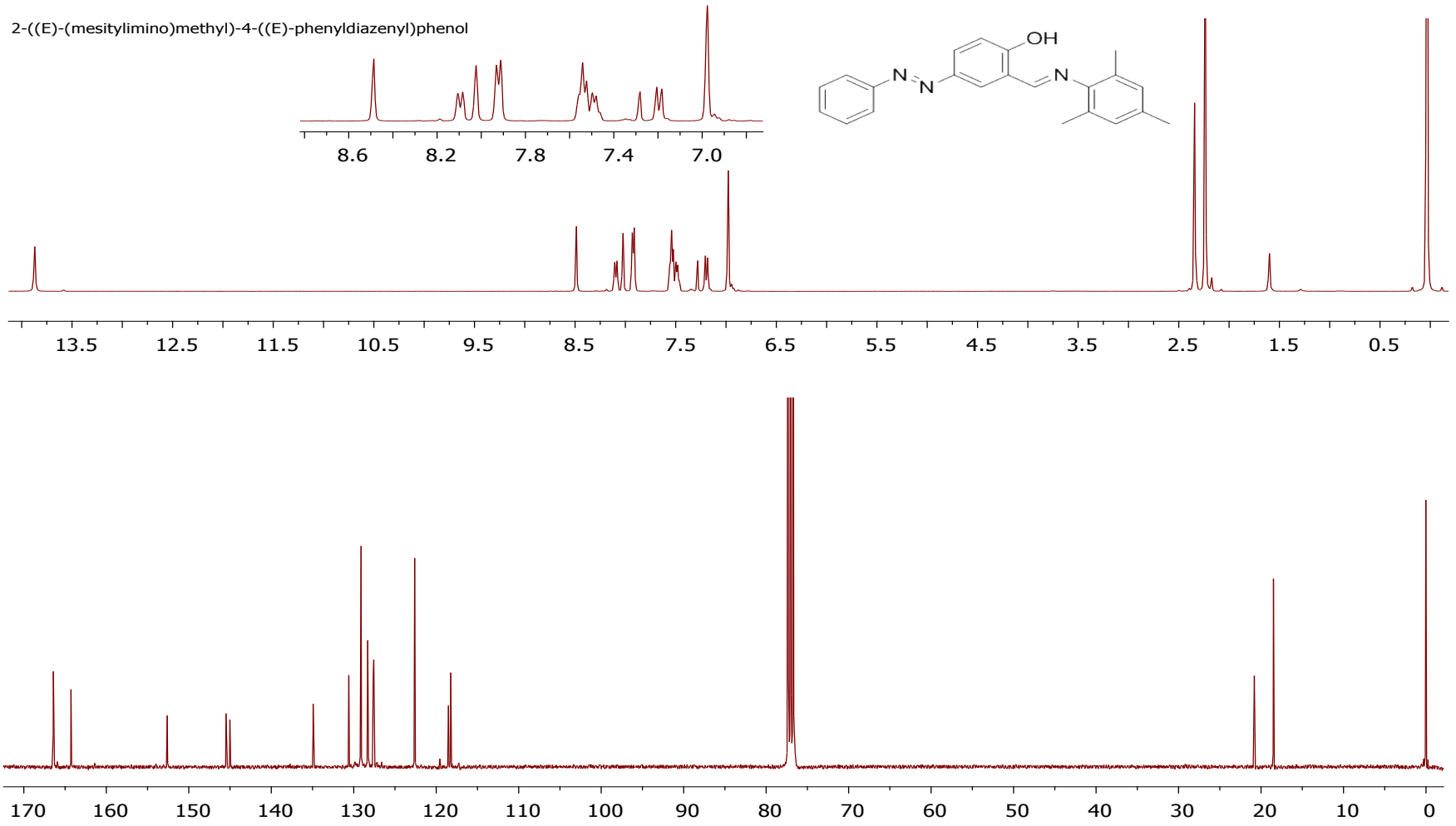

Fig. S5. ^{1}H and ^{13}C-NMR spectrum of **6**

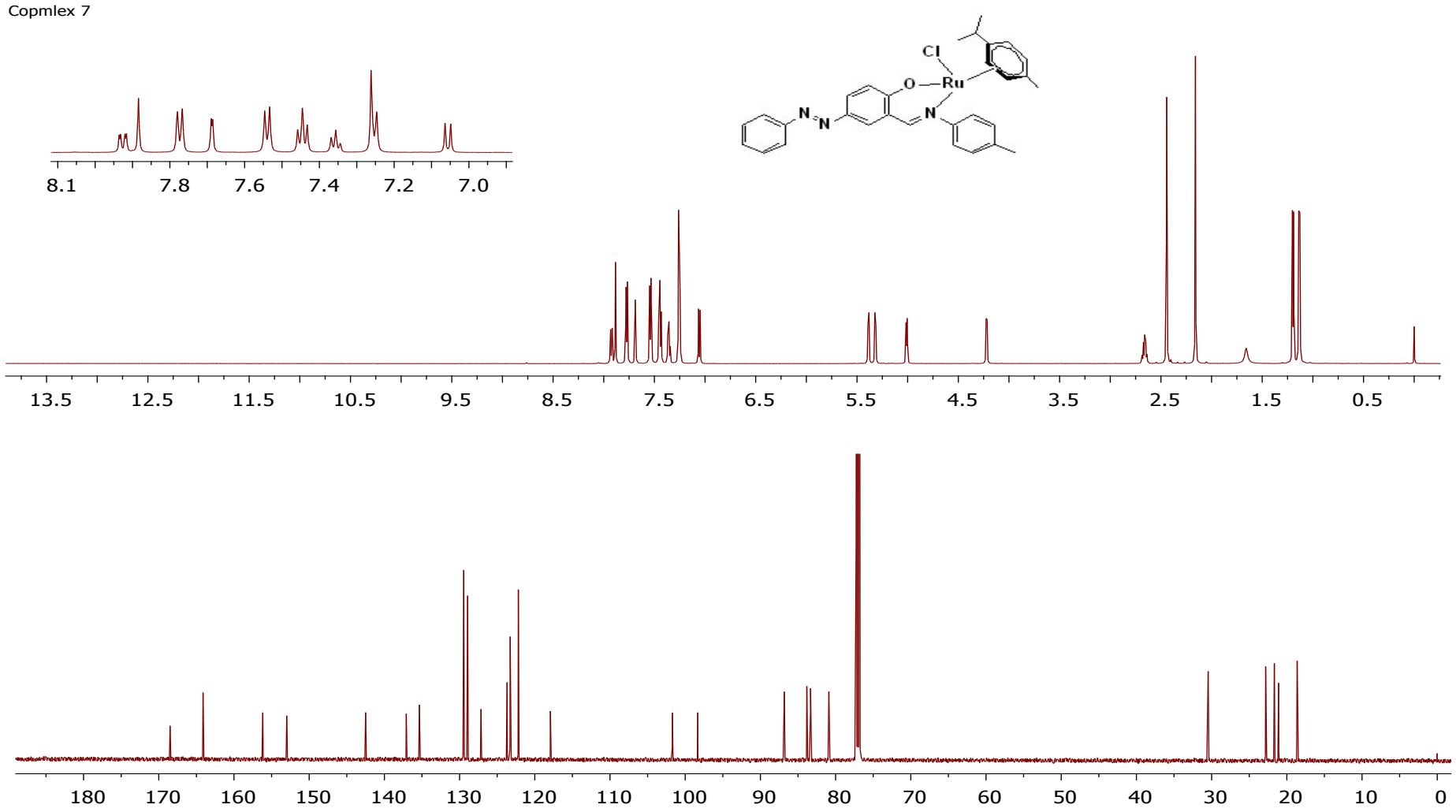

Fig. S6. ^{1}H and ^{13}C-NMR spectrum of **7**

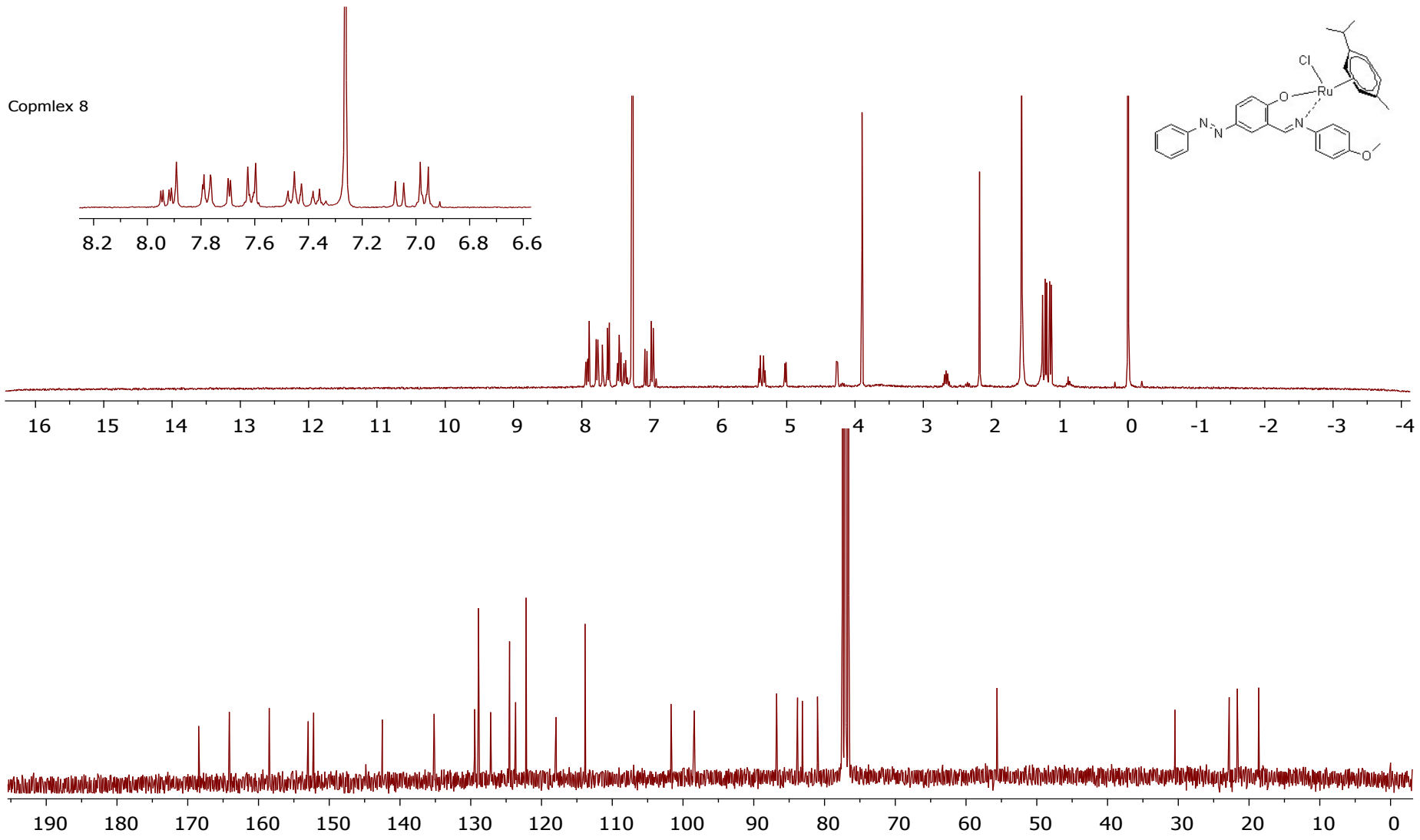

Fig. S7. ^{1}H and ^{13}C-NMR spectrum of **8**

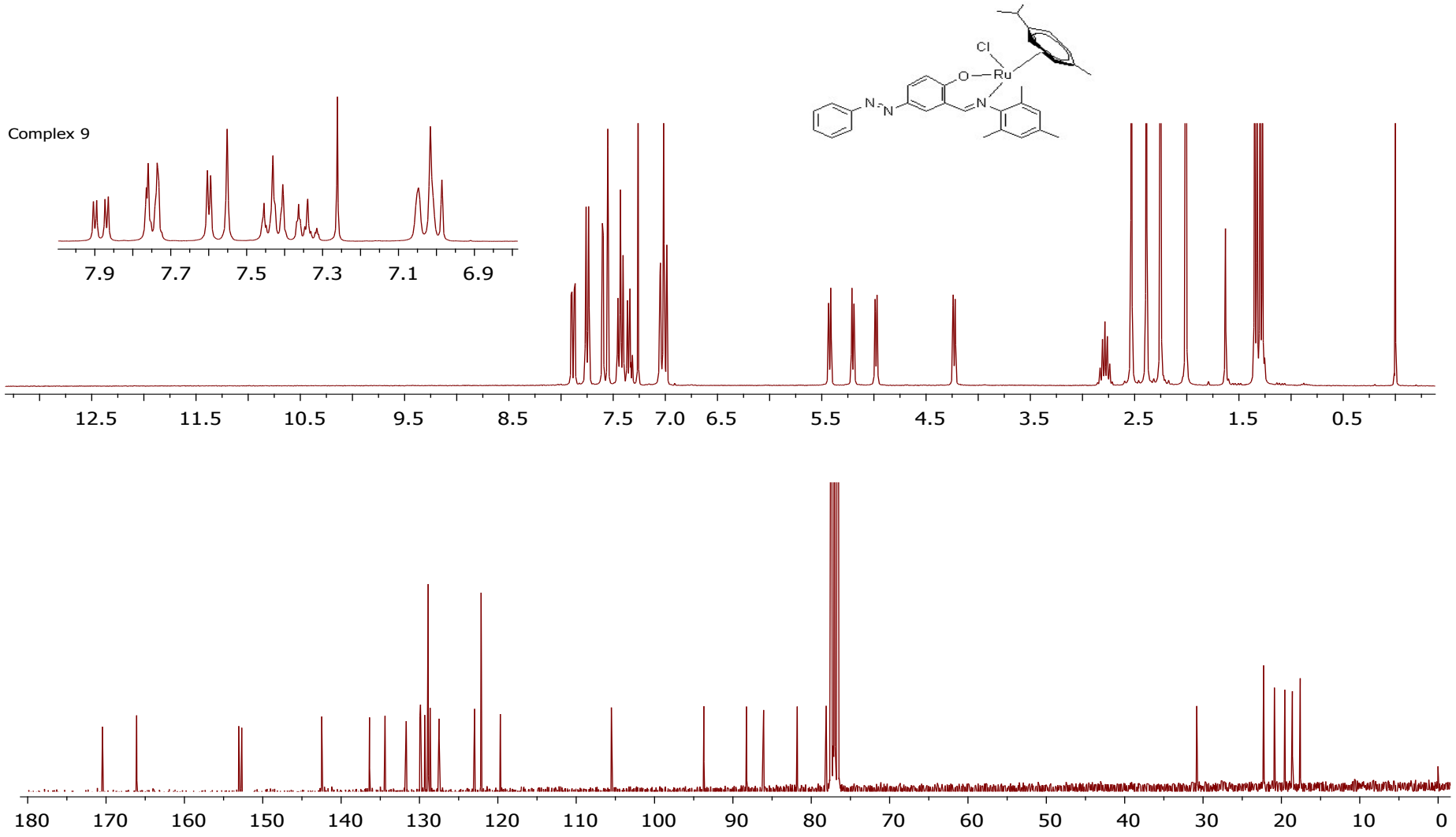

Fig. S8. ^{1}H and ^{13}C-NMR spectrum of **9**

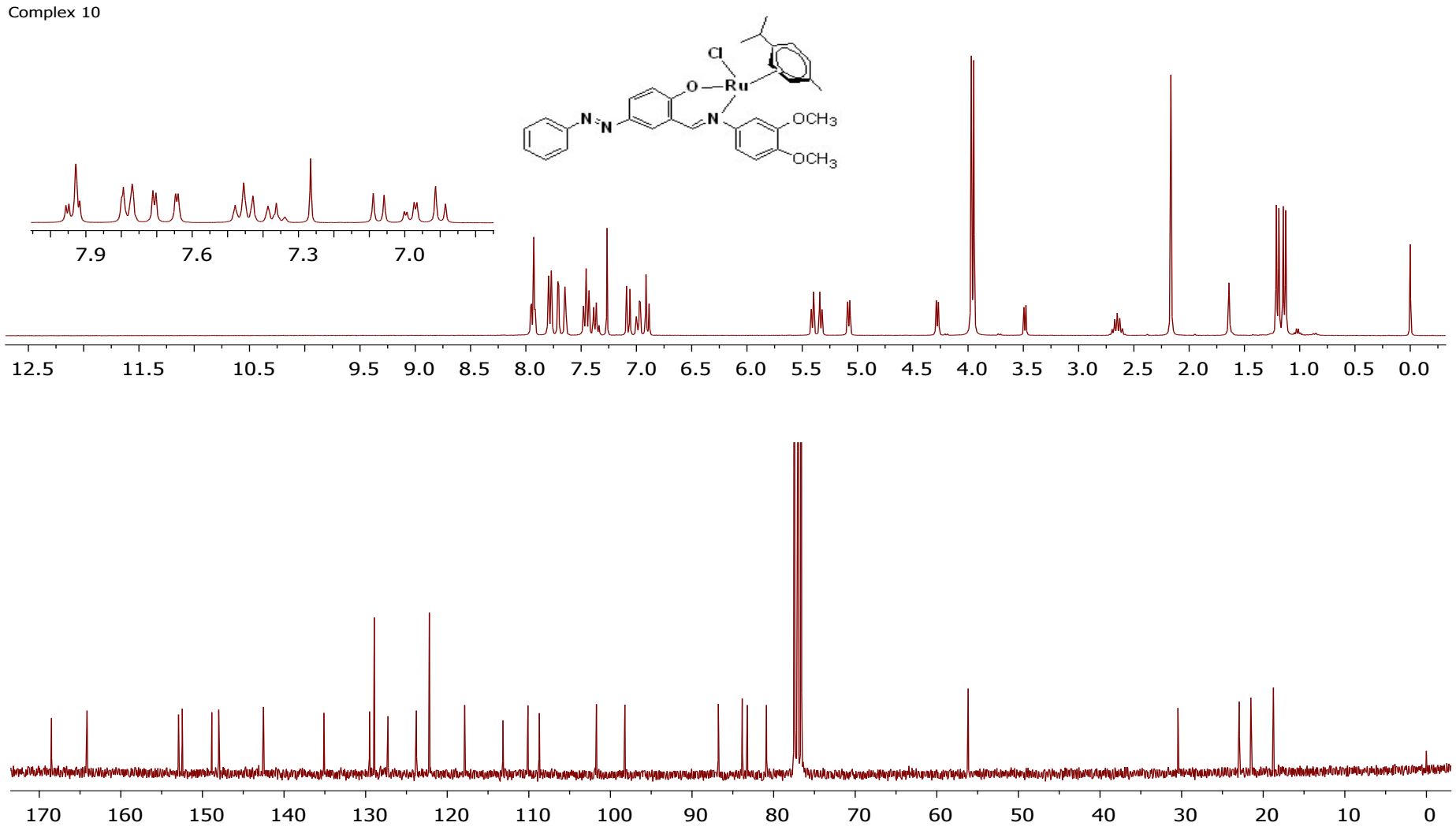

Fig. S9. ^{1}H and ^{13}C-NMR spectrum of **10**

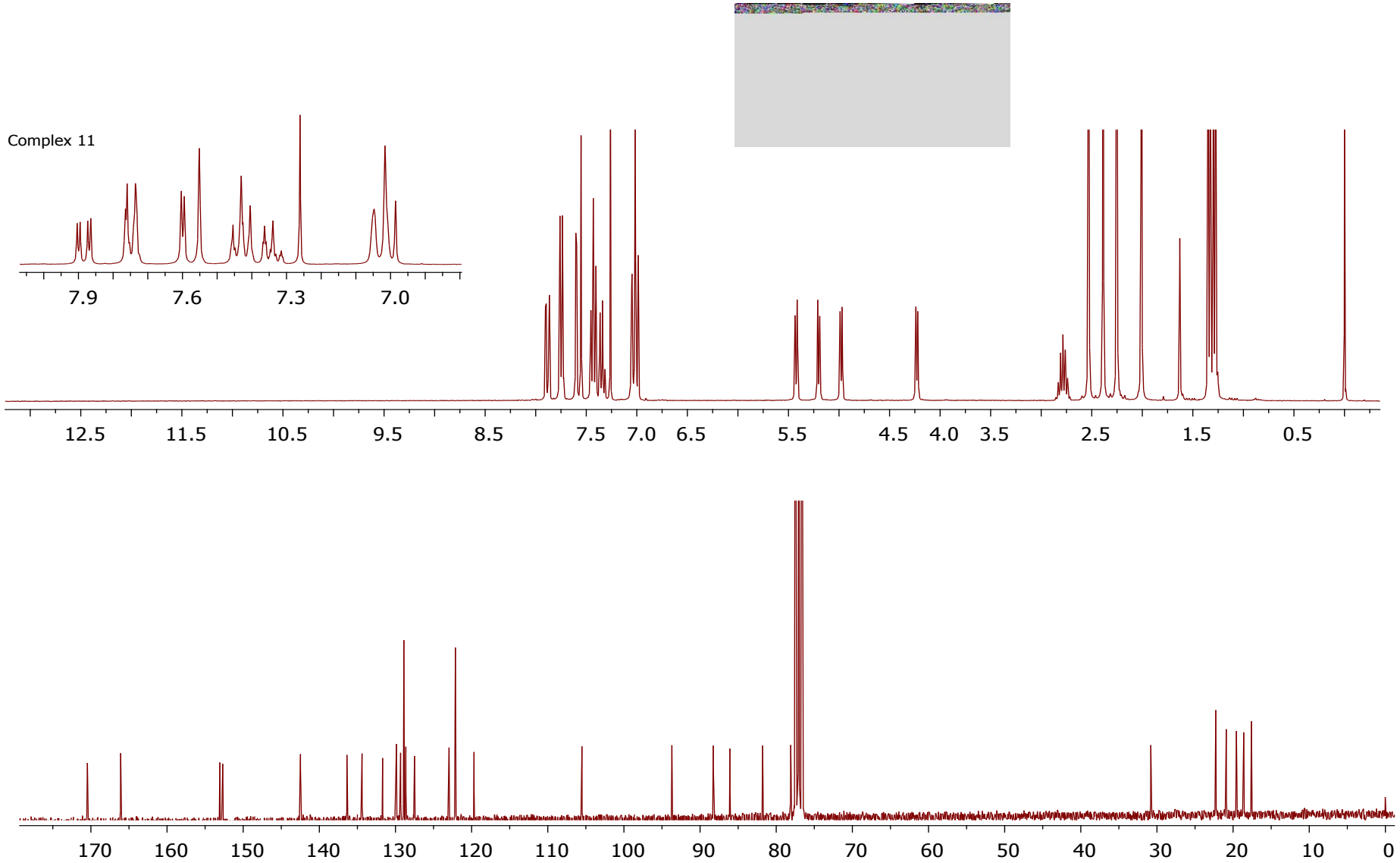

Fig. S10. ^{1}H and ^{13}C-NMR spectrum of **11**

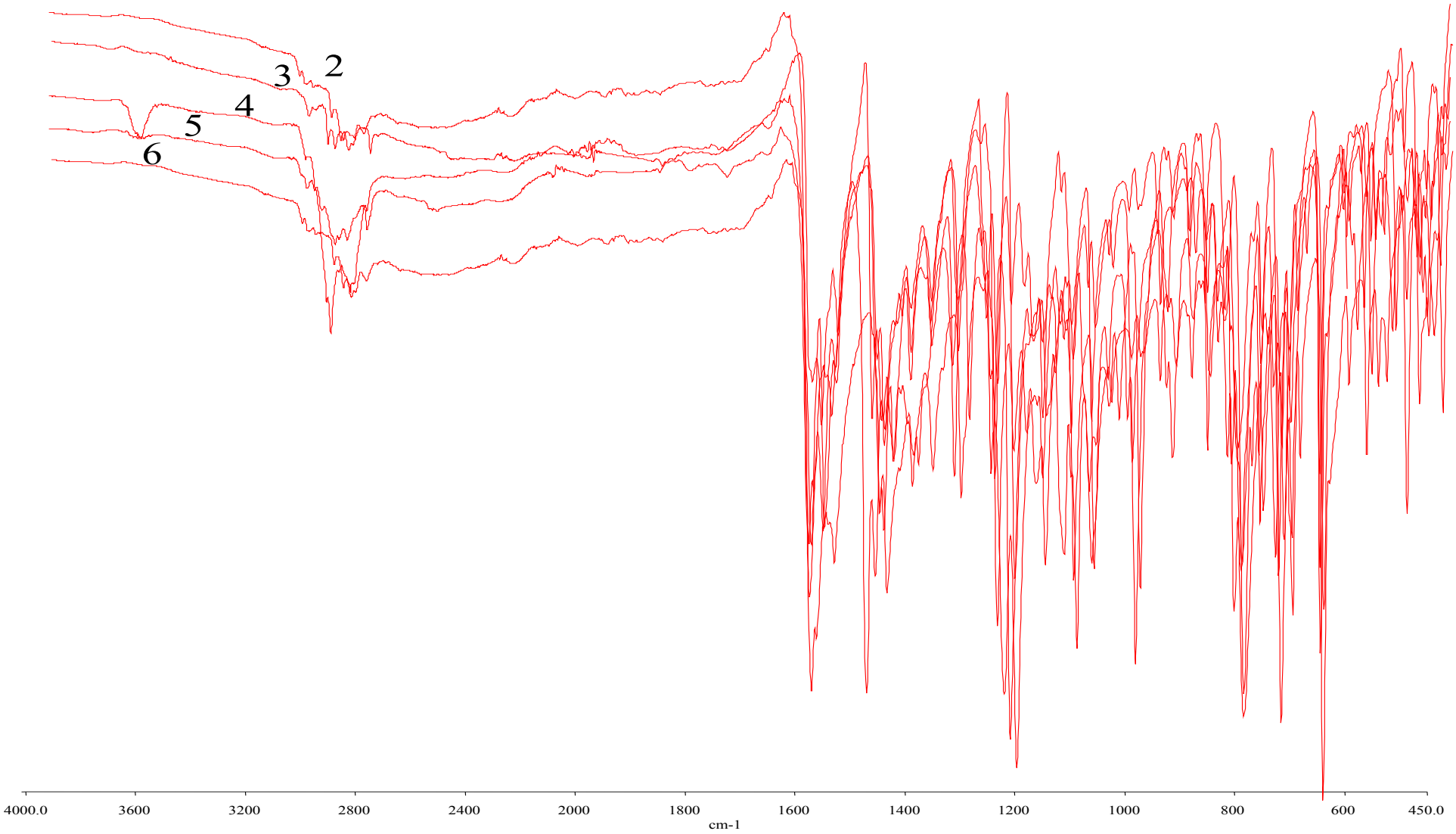

Fig. S11. IR spectrum of ligands (**2-6**)

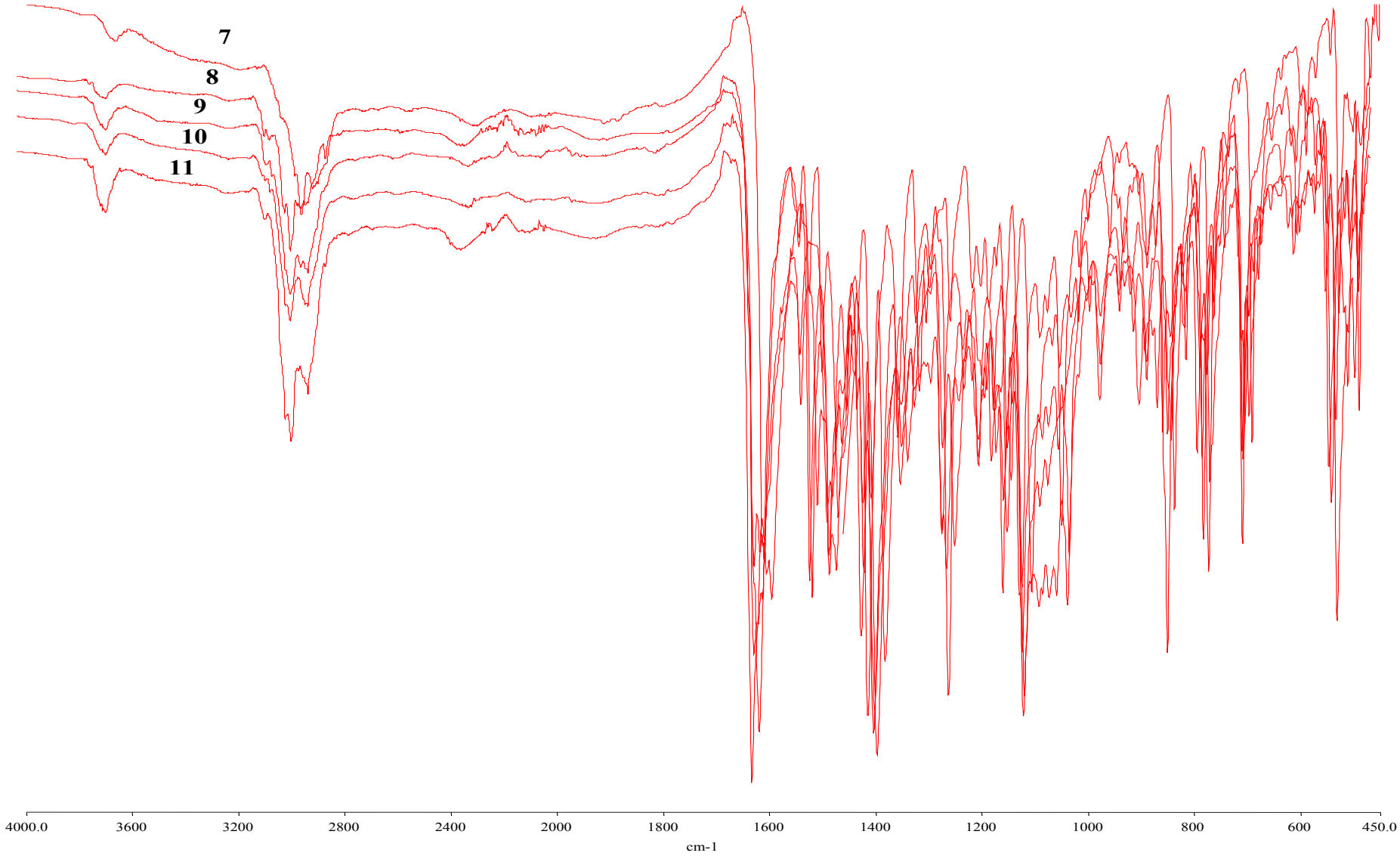

Fig. S12. IR spectrum of complexes (**7-11**)

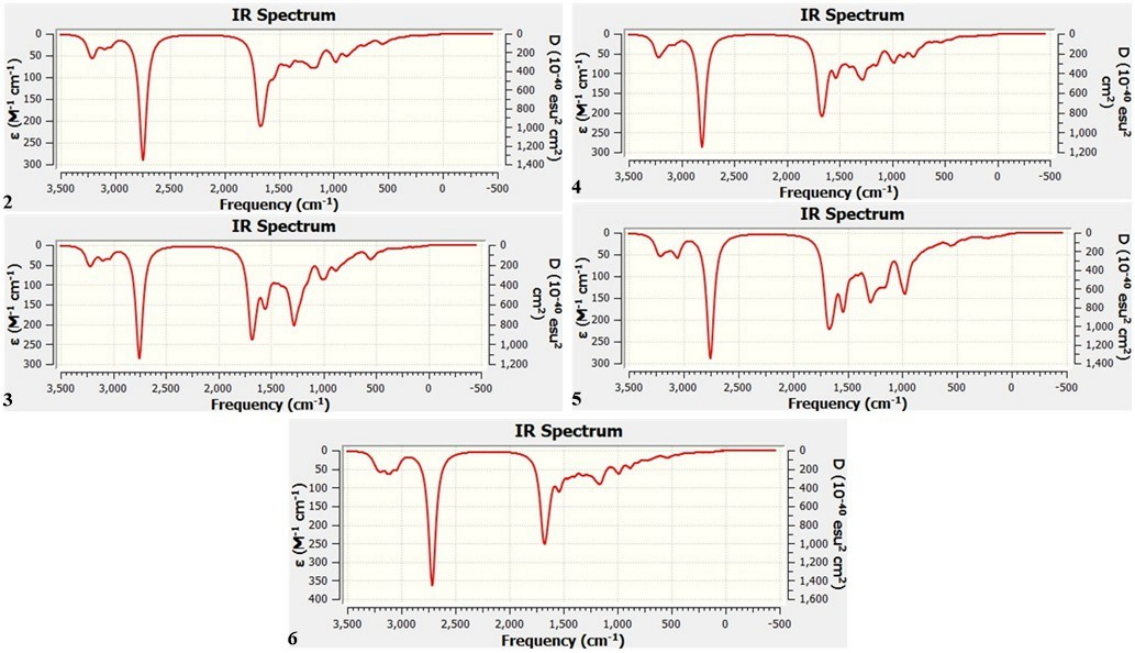

Fig. S13. Calculated IR spectrum of mentioned ligands at same level of theory in gas phase.

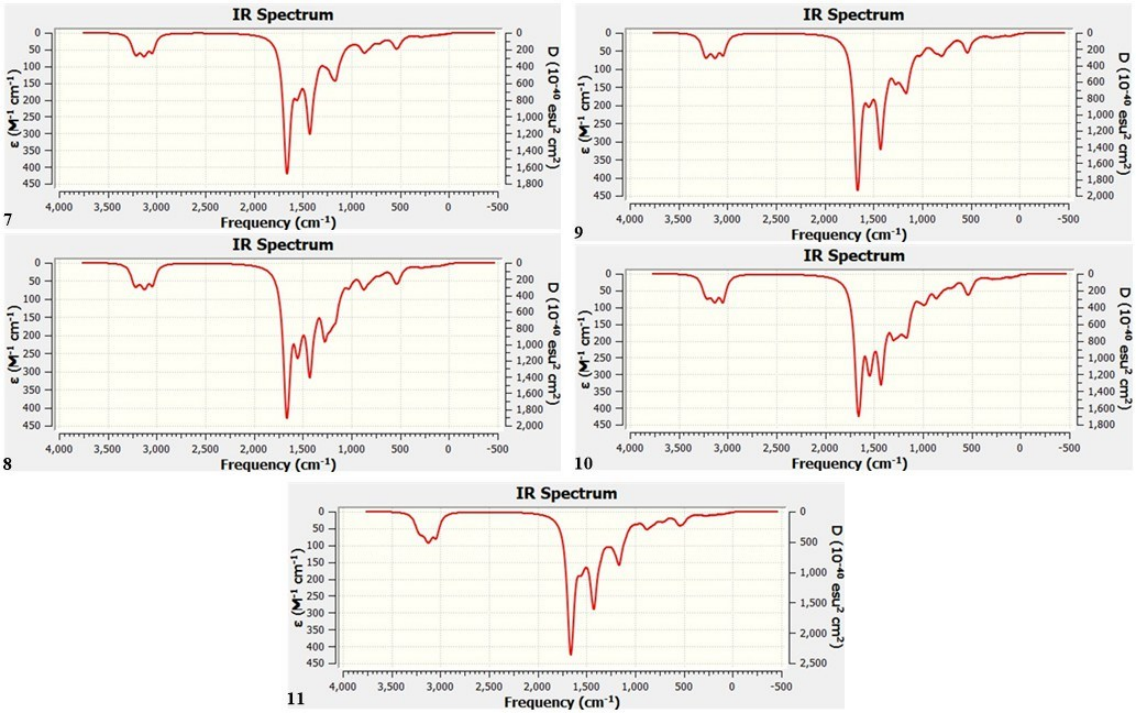

Fig. S14. Calculated IR spectrum of mentioned complexes at same level of theory in gas phase.

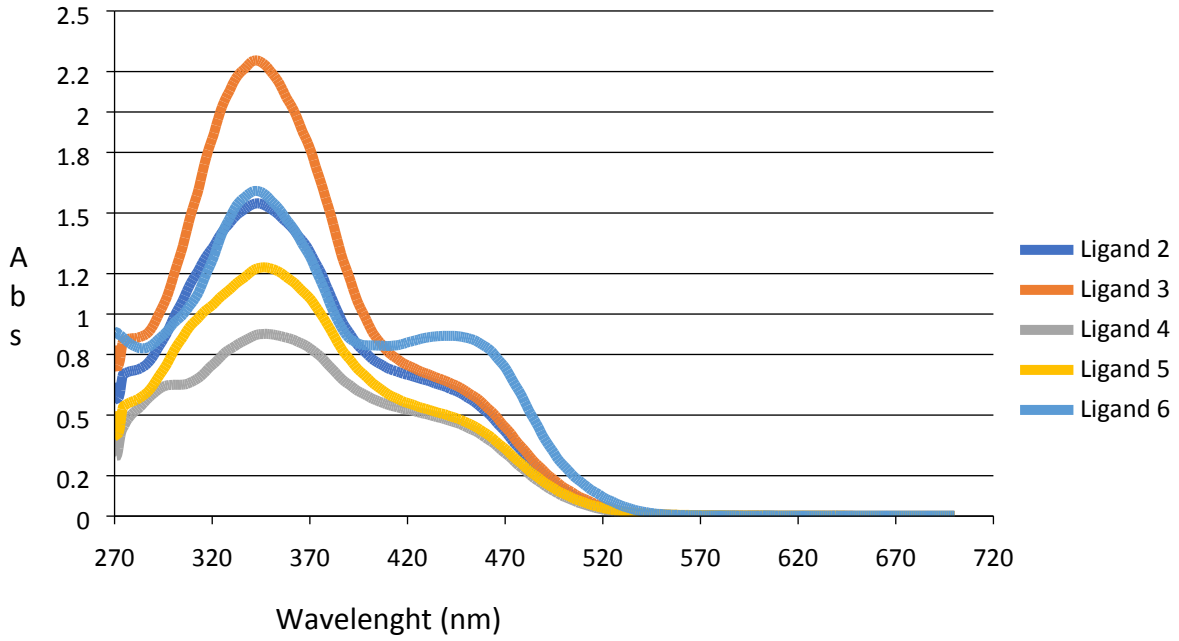

Fig. S15 UV spectrum of ligands (**2-6**)

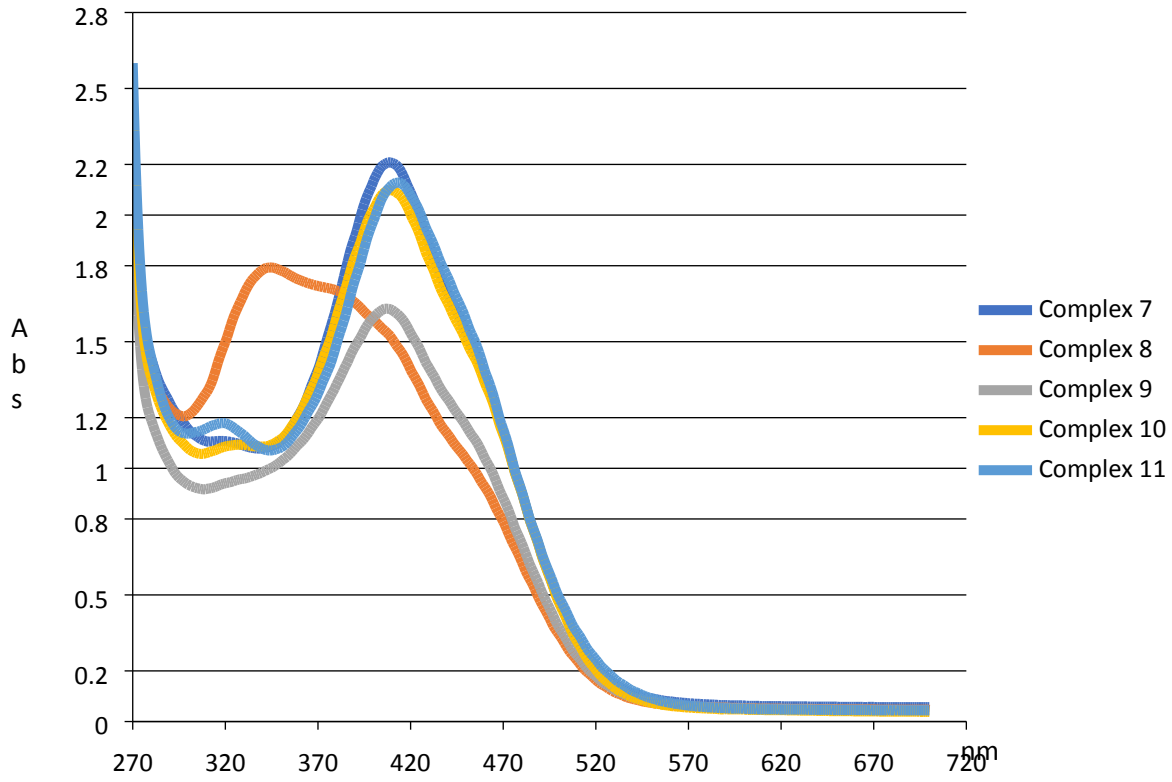

Fig. S16. UV spectrum of complexes (**7-11**)

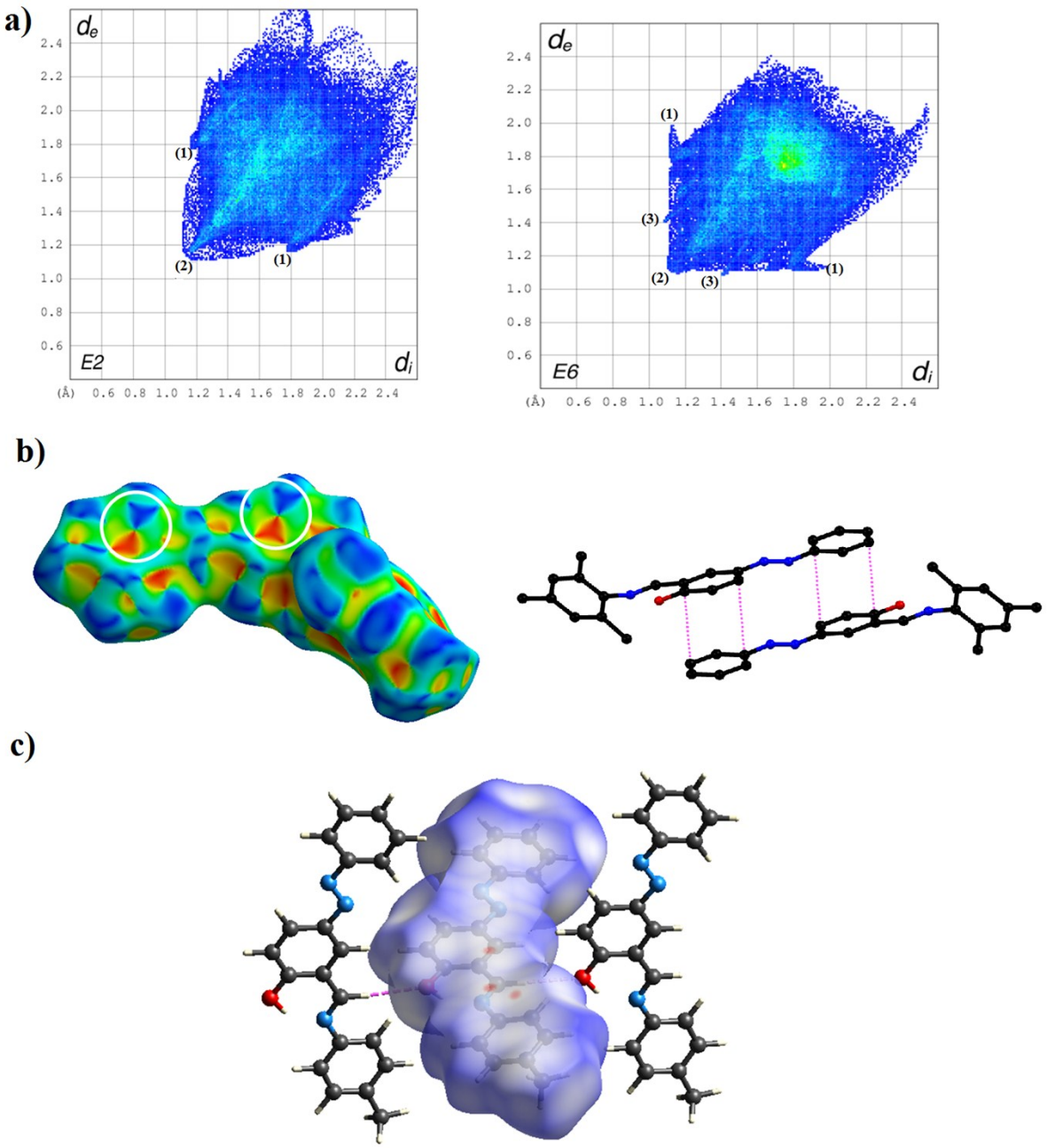

Fig. S17 a) Fingerprint plots b) π-π stacking contacts in **2**

c) CH···O (phenol) hydrogen bond type interactions in **6**.

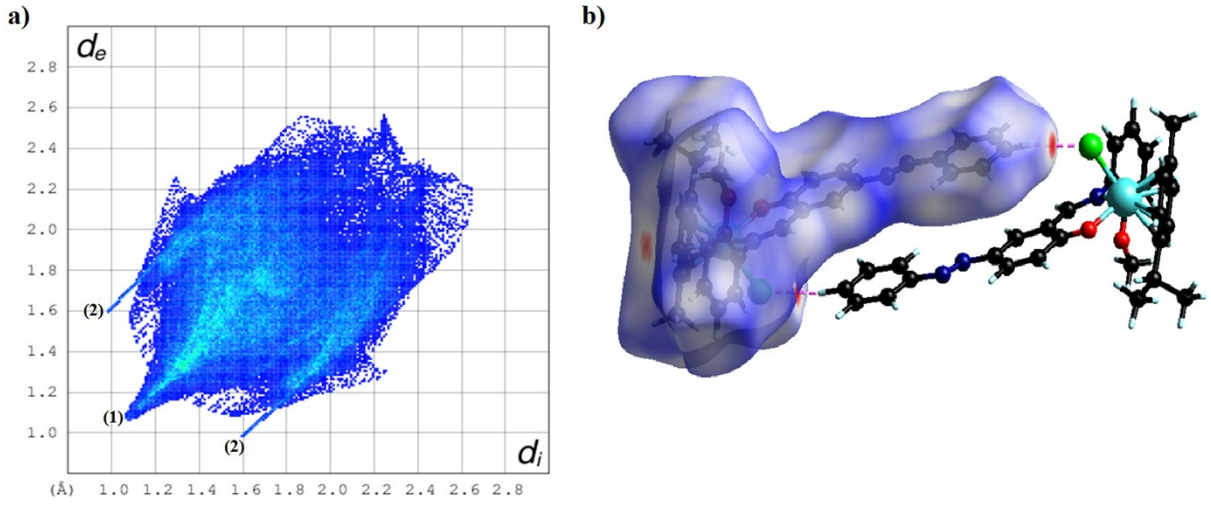

Fig. S18 a) Fingerprint plot of **9** b) d_{norm} surface of **9** showing CH···Cl interactions

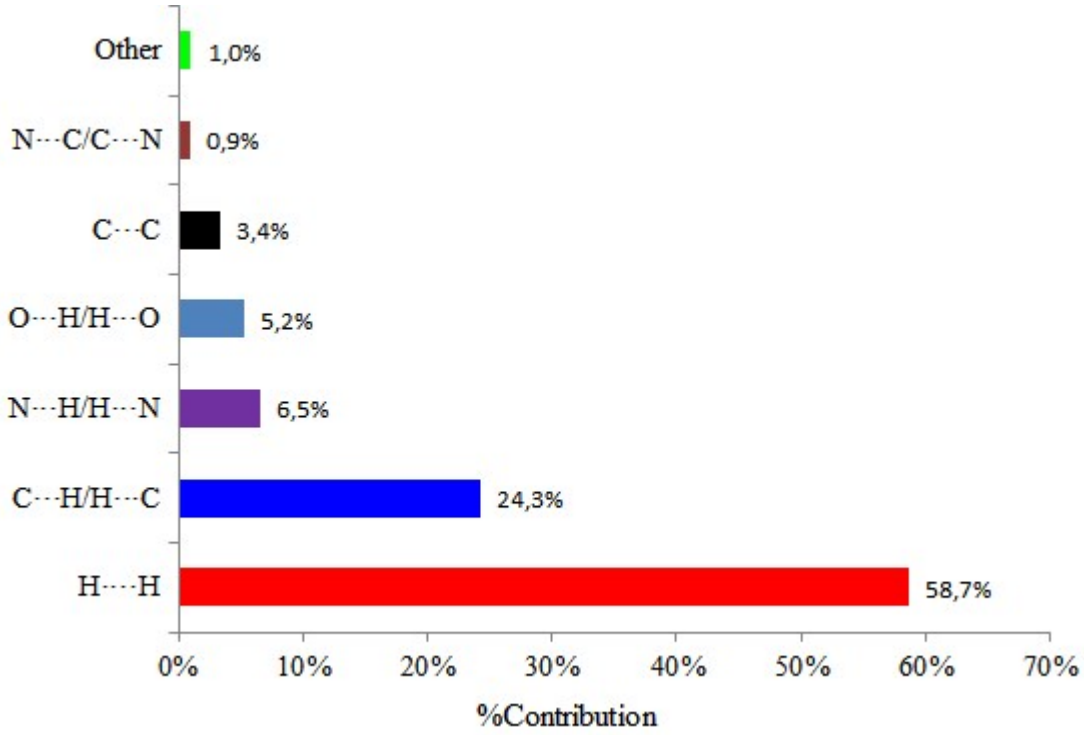

Fig. S19. Percentage contributions of different intermolecular interactions in **2**.

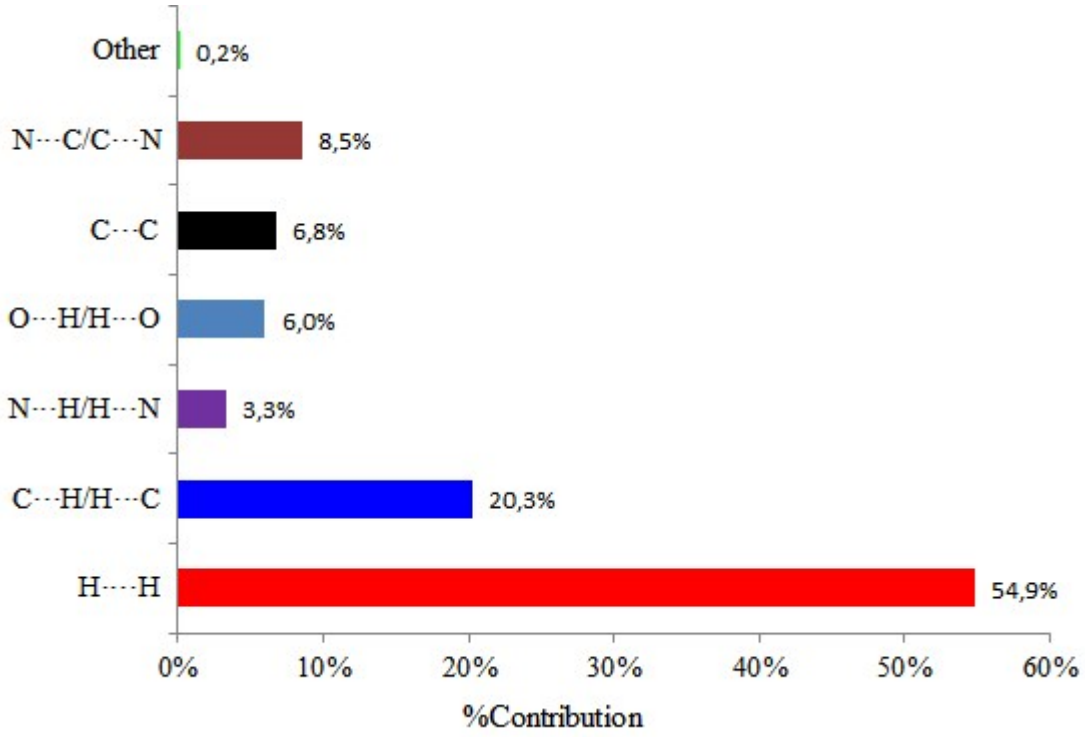

Fig. S20. Percentage contributions of different intermolecular interactions in **6**.

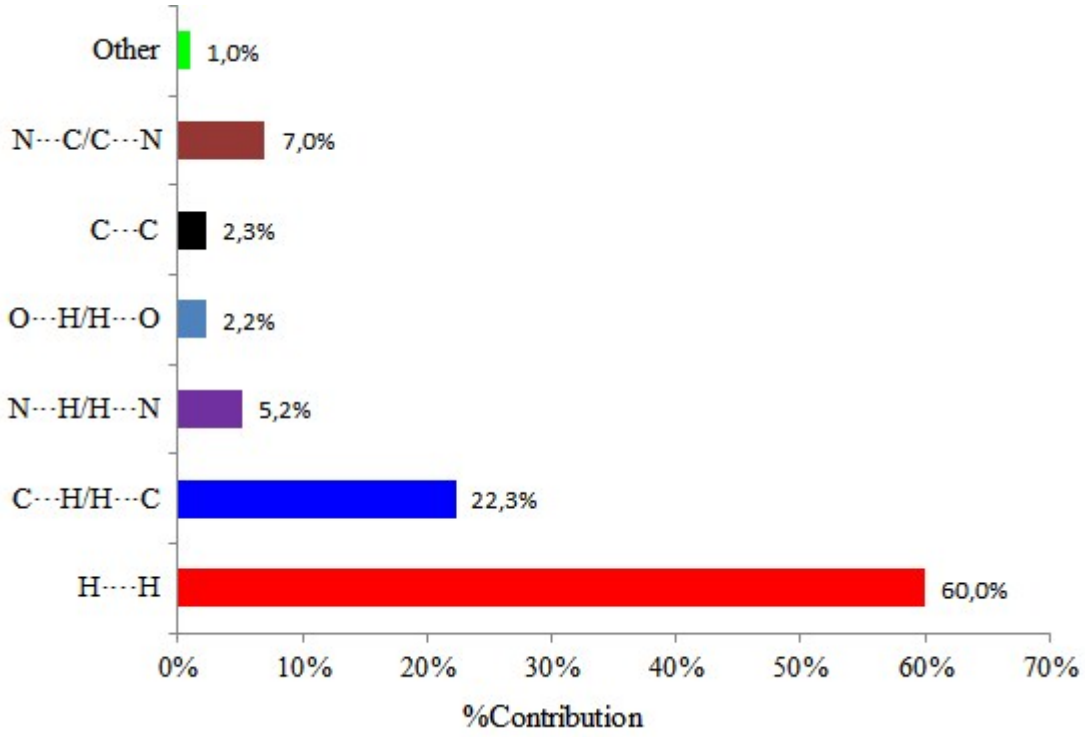

Fig. S21. Percentage contributions of different intermolecular interactions in **10**.

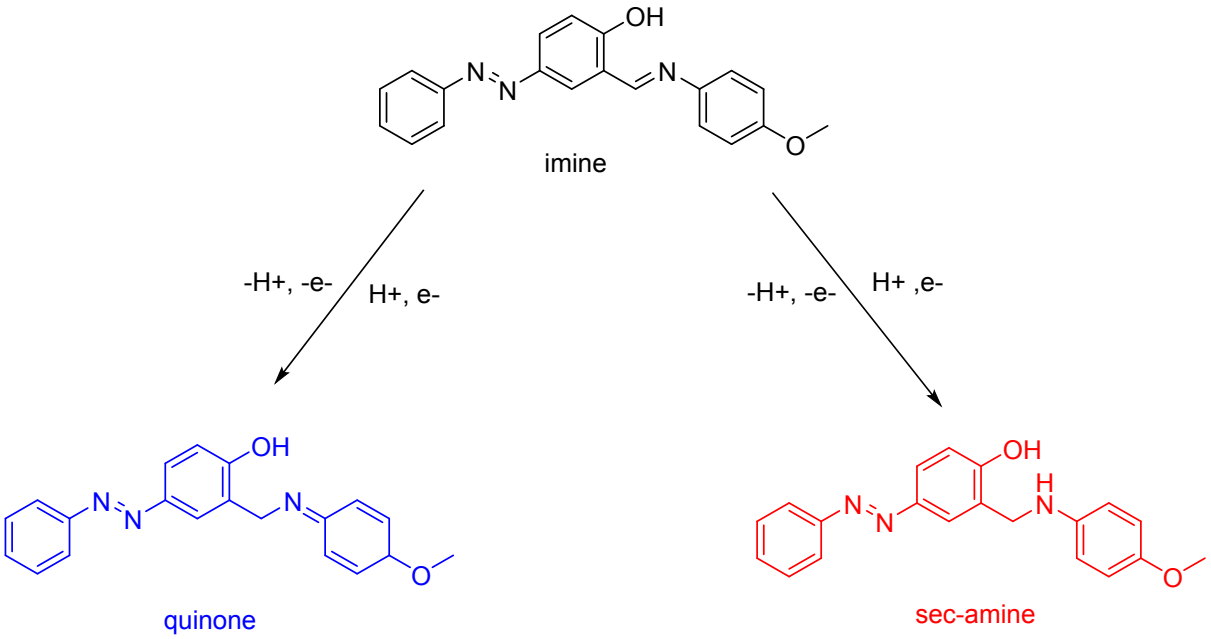

Fig. S22. Reversible reduction–oxidation processes of the new azo Schiff base ligands in DMF solution.

Table S1.

Calculated chemical shift values of carbon atoms in related complexes.

Assignments	**7**	**8**	**9**	**10**	**11**
C1	19.08	19.23	18.91	19.47	18.58
C2	96.69	92.96	95.70	90.04	101.84
C3	102.63	105.41	103.42	104.34	96.91
C4	91.87	87.89	90.93	84.17	97.16
C5	121.36	124.98	121.05	129.65	115.27
C6	84.65	81.92	84.09	77.50	88.06
C7	90.46	93.99	89.90	100.92	89.08
C8	33.06	33.74	33.01	35.76	31.93
C9	25.64	25.64	25.55	26.84	25.38
C10	19.31	19.45	19.11	19.65	18.97
C11	159.08	158.89	161.29	158.85	161.36
C12	116.94	116.81	116.85	116.40	119.81
C13	166.89	166.78	166.98	166.93	168.59
C14	121.90	121.85	121.94	121.95	121.71
C15	116.57	116.55	116.46	116.66	116.36
C16	140.84	140.91	140.76	140.90	141.08
C17	139.19	139.18	139.45	139.33	138.61
C18	148.50	148.46	148.48	148.47	148.51
C19	128.41	128.40	128.31	128.40	128.45
C20	123.74	123.72	123.73	123.73	123.75
C21	125.20	125.23	124.96	125.28	125.11
C22	123.27	123.31	123.24	123.33	123.28
C23	107.91	107.95	107.94	107.97	107.94
C24	153.95	150.36	145.58	152.76	151.08
C25	117.76	119.08	148.21	110.63	129.00
C26	124.76	113.72	107.24	119.08	124.81
C27	133.44	154.96	122.87	145.68	132.95
C28	125.80	107.29	118.29	151.04	126.77
C29	124.27	125.72	126.48	110.11	132.56
C30	21.89	54.20	55.17	59.29	21.97
C31	-	-	-	55.04	20.53
C32	-	-	-	-	21.63

[a]Atomic labellings are represented in Fig. 5.

Table S2.

Calculated chemical shift values of hydrogen atoms in related complexes.

Assignments	**7**	**8**	**9**	**10**	**11**
C1H'	2.62	2.39	2.59	1.99	1.59
C1H''	2.28	2.30	1.69	2.30	3.16
C1H'''	1.48	1.61	2.25	1.98	2.36
C3H	5.61	5.60	5.58	5.43	5.46
C4H	5.61	5.46	5.52	5.33	5.59
C6H	3.63	3.63	3.55	4.08	3.76
C7H	4.82	4.90	5.26	4.77	4.56
C8H	3.90	3.95	3.88	3.66	3.73
C9H'	1.50	1.58	1.57	1.23	1.35
C9H''	1.55	1.59	1.53	1.47	1.11
C9H'''	1.03	1.10	1.02	1.65	0.66
C10H'	1.19	1.84	1.10	2.67	1.48
C10H''	0.67	0.82	0.58	1.07	0.97
C10H'''	1.54	1.28	1.47	1.38	1.54
C11H	7.85	7.83	7.83	7.86	7.64
C14H	6.90	6.90	6.93	6.93	6.86
C15H	7.90	7.90	7.92	7.91	7.86
C17H	7.08	7.08	7.07	7.07	7.02
C19H	7.83	7.84	7.82	7.84	7.80
C20H	7.43	7.44	7.43	7.45	7.44
C21H	7.24	7.23	7.25	7.22	7.27
C22H	7.21	7.21	7.20	7.20	7.21
C23H	7.77	7.78	7.76	7.77	7.75
C25H	7.11	7.14	-	6.75	-
C26H	7.15	7.00	6.68	7.02	6.98
C27H	-	-	7.23	-	-
C28H	7.39	6.62	7.10	-	7.11
C29H	8.49	8.62	8.53	7.93	-
C30H'	1.91	3.77	4.08	5.23	2.14
C30H''	2.62	3.76	4.32	3.43	2.25
C30H'''	2.62	4.20	3.80	4.02	2.61
C31H'	-	-	-	3.87	1.95
C31H''	-	-	-	3.97	2.31
C31H'''	-	-	-	4.21	2.80
C32H'	-	-	-	-	4.06
C32H''	-	-	-	-	1.86
C32H'''	-	-	-	-	2.27

[a]Atomic labellings are represented in Fig. 5.

Table S3.

Selected bond lengths [Å] and angles [°] for ligand **2** –**6**

Assignments	**2**		**3**	**4**	**5**	**6**	
	Experimental	Calculated	Calculated	Calculated	Calculated	Experimental	Calculated
N(1)-N(2)	1.253(2)	1.280	1.281	1.280	1.280	1.259(3)	1.280
N(3)-C(13)	1.279(2)	1.305	1.305	1.305	1.305	1.286(3)	1.303
O(1)-C(10)	1.349(2)	1.356	1.356	1.360	1.356	1.341(3)	1.356
N(1)-C(6)	1.431(2)	1.424	1.424	1.424	1.424	1.425(3)	1.424
N(2)-C(7)	1.423(2)	1.416	1.416	1.417	1.416	1.428(3)	1.416
N(3)-C(14)	1.436(2)	1.417	1.415	1.419	1.416	1.417(3)	1.423
N(2)-N(1)-C(6)	113.82(16)	115.74	115.73	115.80	115.70	115.20(2)	115.70
N(1)-N(2)-C(7)	114.53(16)	115.86	115.88	115.80	115.90	113.23(19)	115.90
C(13)-N(3)-C(14)	118.73(16)	123.33	123.65	121.30	123.50	123.12(19)	

Table S4.

Hydrogen bond parameters for **2** and **6** [Å and °].

	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
2	O(1)-H(1A)...N(3)	0.82	1.76	2.612(2)	146.0
6	O(1)-H(1A)...N(3)	0.82	1.84	2.567(2)	147.4
	C(13)-H(13)...O(1)*	0.93	2.63	3.517(3)	160.4

Symmetrycode* x,-y+3/2,z+1/2

Table S5.
Bond lengths [Å] and angles [°] for **2**.

N(1)-N(2)	1.253(2)	C(11)-C(12)	1.393(2)
N(1)-C(6)	1.431(2)	C(11)-C(13)	1.453(2)
O(1)-C(10)	1.349(2)	C(12)-H(12)	0.9300
O(1)-H(1A)	0.96(3)	C(13)-H(13)	0.9300
C(1)-C(6)	1.383(3)	C(14)-C(19)	1.393(3)
C(1)-C(2)	1.386(3)	C(14)-C(15)	1.395(3)
C(1)-H(1)	0.9300	C(15)-C(16)	1.396(3)
N(2)-C(7)	1.423(2)	C(15)-C(20)	1.507(3)
C(2)-C(3)	1.370(4)	C(16)-C(17)	1.375(3)
C(2)-H(2)	0.9300	C(16)-H(16)	0.9300
N(3)-C(13)	1.279(2)	C(17)-C(18)	1.377(3)
N(3)-C(14)	1.436(2)	C(17)-C(21)	1.518(3)
C(3)-C(4)	1.379(3)	C(18)-C(19)	1.391(3)
C(3)-H(3)	0.9300	C(18)-H(18)	0.9300
C(4)-C(5)	1.379(3)	C(19)-C(22)	1.503(3)
C(4)-H(4)	0.9300	C(20)-H(20A)	0.9600
C(5)-C(6)	1.388(3)	C(20)-H(20B)	0.9600
C(5)-H(5)	0.9300	C(20)-H(20C)	0.9600
C(7)-C(12)	1.381(2)	C(21)-H(21A)	0.9600
C(7)-C(8)	1.401(3)	C(21)-H(21B)	0.9600
C(8)-C(9)	1.370(3)	C(21)-H(21C)	0.9600
C(8)-H(8)	0.9300	C(22)-H(22A)	0.9600
C(9)-C(10)	1.393(2)	C(22)-H(22B)	0.9600
C(9)-H(9)	0.9300	C(22)-H(22C)	0.9600
C(10)-C(11)	1.409(3)		

N(2)-N(1)-C(6)	113.82(16)	C(3)-C(2)-H(2)	119.6
C(10)-O(1)-H(1A)	108.6(17)	C(1)-C(2)-H(2)	119.6
C(6)-C(1)-C(2)	119.1(2)	C(13)-N(3)-C(14)	118.73(16)
C(6)-C(1)-H(1)	120.4	C(2)-C(3)-C(4)	119.8(2)
C(2)-C(1)-H(1)	120.4	C(2)-C(3)-H(3)	120.1
N(1)-N(2)-C(7)	114.53(16)	C(4)-C(3)-H(3)	120.1
C(3)-C(2)-C(1)	120.9(2)	C(3)-C(4)-C(5)	120.3(2)

C(3)-C(4)-H(4)	119.9	C(14)-C(15)-C(20)	123.06(19)
C(5)-C(4)-H(4)	119.9	C(16)-C(15)-C(20)	119.1(2)
C(4)-C(5)-C(6)	119.68(19)	C(17)-C(16)-C(15)	122.2(2)
C(4)-C(5)-H(5)	120.2	C(17)-C(16)-H(16)	118.9
C(6)-C(5)-H(5)	120.2	C(15)-C(16)-H(16)	118.9
C(1)-C(6)-C(5)	120.23(18)	C(16)-C(17)-C(18)	118.34(19)
C(1)-C(6)-N(1)	115.59(18)	C(16)-C(17)-C(21)	121.1(2)
C(5)-C(6)-N(1)	124.17(16)	C(18)-C(17)-C(21)	120.6(2)
C(12)-C(7)-C(8)	119.48(16)	C(17)-C(18)-C(19)	122.2(2)
C(12)-C(7)-N(2)	116.09(16)	C(17)-C(18)-H(18)	118.9
C(8)-C(7)-N(2)	124.43(15)	C(19)-C(18)-H(18)	118.9
C(9)-C(8)-C(7)	120.63(16)	C(18)-C(19)-C(14)	118.1(2)
C(9)-C(8)-H(8)	119.7	C(18)-C(19)-C(22)	120.7(2)
C(7)-C(8)-H(8)	119.7	C(14)-C(19)-C(22)	121.15(18)
C(8)-C(9)-C(10)	120.02(17)	C(15)-C(20)-H(20A)	109.5
C(8)-C(9)-H(9)	120.0	C(15)-C(20)-H(20B)	109.5
C(10)-C(9)-H(9)	120.0	H(20A)-C(20)-H(20B)	109.5
O(1)-C(10)-C(9)	118.55(17)	C(15)-C(20)-H(20C)	109.5
O(1)-C(10)-C(11)	121.25(16)	H(20A)-C(20)-H(20C)	109.5
C(9)-C(10)-C(11)	120.20(16)	H(20B)-C(20)-H(20C)	109.5
C(12)-C(11)-C(10)	118.66(15)	C(17)-C(21)-H(21A)	109.5
C(12)-C(11)-C(13)	119.70(16)	C(17)-C(21)-H(21B)	109.5
C(10)-C(11)-C(13)	121.63(16)	H(21A)-C(21)-H(21B)	109.5
C(7)-C(12)-C(11)	120.98(17)	C(17)-C(21)-H(21C)	109.5
C(7)-C(12)-H(12)	119.5	H(21A)-C(21)-H(21C)	109.5
C(11)-C(12)-H(12)	119.5	H(21B)-C(21)-H(21C)	109.5
N(3)-C(13)-C(11)	122.02(18)	C(19)-C(22)-H(22A)	109.5
N(3)-C(13)-H(13)	119.0	C(19)-C(22)-H(22B)	109.5
C(11)-C(13)-H(13)	119.0	H(22A)-C(22)-H(22B)	109.5
C(19)-C(14)-C(15)	121.26(17)	C(19)-C(22)-H(22C)	109.5
C(19)-C(14)-N(3)	117.72(18)	H(22A)-C(22)-H(22C)	109.5
C(15)-C(14)-N(3)	120.97(18)	H(22B)-C(22)-H(22C)	109.5
C(14)-C(15)-C(16)	117.8(2)		

Table S6.

Torsion angles [°] for **2**.

C(6)-N(1)-N(2)-C(7)	179.33(15)
C(6)-C(1)-C(2)-C(3)	-0.3(3)
C(1)-C(2)-C(3)-C(4)	0.3(4)
C(2)-C(3)-C(4)-C(5)	-0.2(4)
C(3)-C(4)-C(5)-C(6)	0.2(3)
C(2)-C(1)-C(6)-C(5)	0.3(3)
C(2)-C(1)-C(6)-N(1)	-179.24(18)
C(4)-C(5)-C(6)-C(1)	-0.2(3)
C(4)-C(5)-C(6)-N(1)	179.28(19)
N(2)-N(1)-C(6)-C(1)	177.55(17)
N(2)-N(1)-C(6)-C(5)	-1.9(3)
N(1)-N(2)-C(7)-C(12)	177.20(16)
N(1)-N(2)-C(7)-C(8)	-2.9(3)
C(12)-C(7)-C(8)-C(9)	-0.5(3)
N(2)-C(7)-C(8)-C(9)	179.55(18)
C(7)-C(8)-C(9)-C(10)	0.6(3)
C(8)-C(9)-C(10)-O(1)	179.04(18)
C(8)-C(9)-C(10)-C(11)	-1.0(3)
O(1)-C(10)-C(11)-C(12)	-178.71(17)
C(9)-C(10)-C(11)-C(12)	1.3(3)
O(1)-C(10)-C(11)-C(13)	1.5(3)
C(9)-C(10)-C(11)-C(13)	-178.45(17)
C(8)-C(7)-C(12)-C(11)	0.9(3)
N(2)-C(7)-C(12)-C(11)	-179.19(16)
C(10)-C(11)-C(12)-C(7)	-1.3(3)
C(13)-C(11)-C(12)-C(7)	178.48(17)
C(14)-N(3)-C(13)-C(11)	179.14(17)
C(12)-C(11)-C(13)-N(3)	-178.29(17)
C(10)-C(11)-C(13)-N(3)	1.5(3)
C(13)-N(3)-C(14)-C(19)	111.7(2)
C(13)-N(3)-C(14)-C(15)	-70.6(2)
C(19)-C(14)-C(15)-C(16)	-2.4(3)
N(3)-C(14)-C(15)-C(16)	-179.96(18)
C(19)-C(14)-C(15)-C(20)	175.9(2)
N(3)-C(14)-C(15)-C(20)	-1.7(3)

C(14)-C(15)-C(16)-C(17)	0.1(3)
C(20)-C(15)-C(16)-C(17)	-178.2(2)
C(15)-C(16)-C(17)-C(18)	1.6(4)
C(15)-C(16)-C(17)-C(21)	-178.1(2)
C(16)-C(17)-C(18)-C(19)	-1.1(3)
C(21)-C(17)-C(18)-C(19)	178.5(2)
C(17)-C(18)-C(19)-C(14)	-1.1(3)
C(17)-C(18)-C(19)-C(22)	-179.9(2)
C(15)-C(14)-C(19)-C(18)	2.9(3)
N(3)-C(14)-C(19)-C(18)	-179.51(18)
C(15)-C(14)-C(19)-C(22)	-178.3(2)
N(3)-C(14)-C(19)-C(22)	-0.7(3)

Table S7.

Bond lengths [Å] and angles [°] for **6**.

O(1)-C(10)	1.341(3)	C(9)-C(10)	1.389(3)
O(1)-H(1A)	0.8200	C(9)-H(9)	0.9300
N(1)-N(2)	1.259(3)	C(10)-C(11)	1.411(3)
N(1)-C(6)	1.425(3)	C(11)-C(12)	1.393(3)
C(1)-C(6)	1.383(3)	C(11)-C(13)	1.445(3)
C(1)-C(2)	1.384(4)	C(12)-H(12)	0.9300
C(1)-H(1)	0.9300	C(13)-H(13)	0.9300
N(2)-C(7)	1.428(3)	C(14)-C(19)	1.382(3)
C(2)-C(3)	1.370(4)	C(14)-C(15)	1.385(3)
C(2)-H(2)	0.9300	C(15)-C(16)	1.384(3)
N(3)-C(13)	1.286(3)	C(15)-H(15)	0.9300
N(3)-C(14)	1.417(3)	C(16)-C(17)	1.384(3)
C(3)-C(4)	1.377(4)	C(16)-H(16)	0.9300
C(3)-H(3)	0.9300	C(17)-C(18)	1.380(3)
C(4)-C(5)	1.383(3)	C(17)-C(20)	1.505(3)
C(4)-H(4)	0.9300	C(18)-C(19)	1.381(3)
C(5)-C(6)	1.380(3)	C(18)-H(18)	0.9300
C(5)-H(5)	0.9300	C(19)-H(19)	0.9300
C(7)-C(12)	1.382(3)	C(20)-H(20A)	0.9600
C(7)-C(8)	1.398(3)	C(20)-H(20B)	0.9600
C(8)-C(9)	1.371(3)	C(20)-H(20C)	0.9600
C(8)-H(8)	0.9300		

C(10)-O(1)-H(1A)	109.5	C(2)-C(3)-H(3)	120.0
N(2)-N(1)-C(6)	115.2(2)	C(4)-C(3)-H(3)	120.0
C(6)-C(1)-C(2)	120.5(3)	C(3)-C(4)-C(5)	120.6(3)
C(6)-C(1)-H(1)	119.8	C(3)-C(4)-H(4)	119.7
C(2)-C(1)-H(1)	119.8	C(5)-C(4)-H(4)	119.7
N(1)-N(2)-C(7)	113.23(19)	C(6)-C(5)-C(4)	119.6(2)
C(3)-C(2)-C(1)	119.8(3)	C(6)-C(5)-H(5)	120.2
C(3)-C(2)-H(2)	120.1	C(4)-C(5)-H(5)	120.2
C(1)-C(2)-H(2)	120.1	C(5)-C(6)-C(1)	119.5(2)
C(13)-N(3)-C(14)	123.12(19)	C(5)-C(6)-N(1)	125.5(2)
C(2)-C(3)-C(4)	120.0(3)	C(1)-C(6)-N(1)	115.0(2)

C(12)-C(7)-C(8)	118.7(2)	C(15)-C(14)-N(3)	125.5(2)
C(12)-C(7)-N(2)	117.5(2)	C(16)-C(15)-C(14)	120.5(2)
C(8)-C(7)-N(2)	123.7(2)	C(16)-C(15)-H(15)	119.7
C(9)-C(8)-C(7)	120.6(2)	C(14)-C(15)-H(15)	119.7
C(9)-C(8)-H(8)	119.7	C(15)-C(16)-C(17)	121.8(2)
C(7)-C(8)-H(8)	119.7	C(15)-C(16)-H(16)	119.1
C(8)-C(9)-C(10)	120.7(2)	C(17)-C(16)-H(16)	119.1
C(8)-C(9)-H(9)	119.7	C(18)-C(17)-C(16)	117.3(2)
C(10)-C(9)-H(9)	119.7	C(18)-C(17)-C(20)	121.7(2)
O(1)-C(10)-C(9)	118.4(2)	C(16)-C(17)-C(20)	121.0(2)
O(1)-C(10)-C(11)	121.7(2)	C(17)-C(18)-C(19)	121.1(2)
C(9)-C(10)-C(11)	119.9(2)	C(17)-C(18)-H(18)	119.4
C(12)-C(11)-C(10)	118.10(19)	C(19)-C(18)-H(18)	119.4
C(12)-C(11)-C(13)	121.18(19)	C(18)-C(19)-C(14)	121.6(2)
C(10)-C(11)-C(13)	120.72(19)	C(18)-C(19)-H(19)	119.2
C(7)-C(12)-C(11)	122.0(2)	C(14)-C(19)-H(19)	119.2
C(7)-C(12)-H(12)	119.0	C(17)-C(20)-H(20A)	109.5
C(11)-C(12)-H(12)	119.0	C(17)-C(20)-H(20B)	109.5
N(3)-C(13)-C(11)	121.2(2)	H(20A)-C(20)-H(20B)	109.5
N(3)-C(13)-H(13)	119.4	C(17)-C(20)-H(20C)	109.5
C(11)-C(13)-H(13)	119.4	H(20A)-C(20)-H(20C)	109.5
C(19)-C(14)-C(15)	117.6(2)	H(20B)-C(20)-H(20C)	109.5
C(19)-C(14)-N(3)	116.84(19)		

Table S8.

Torsion angles [°] for **6**.

C(6)-N(1)-N(2)-C(7)	-177.78(17)
C(6)-C(1)-C(2)-C(3)	0.9(4)
C(1)-C(2)-C(3)-C(4)	0.1(4)
C(2)-C(3)-C(4)-C(5)	-0.8(4)
C(3)-C(4)-C(5)-C(6)	0.7(4)
C(4)-C(5)-C(6)-C(1)	0.2(4)
C(4)-C(5)-C(6)-N(1)	178.4(2)
C(2)-C(1)-C(6)-C(5)	-1.0(4)
C(2)-C(1)-C(6)-N(1)	-179.4(2)
N(2)-N(1)-C(6)-C(5)	2.7(3)
N(2)-N(1)-C(6)-C(1)	-179.1(2)
N(1)-N(2)-C(7)-C(12)	-173.74(19)
N(1)-N(2)-C(7)-C(8)	8.3(3)
C(12)-C(7)-C(8)-C(9)	-0.7(3)
N(2)-C(7)-C(8)-C(9)	177.2(2)
C(7)-C(8)-C(9)-C(10)	-0.1(4)
C(8)-C(9)-C(10)-O(1)	-178.3(2)
C(8)-C(9)-C(10)-C(11)	0.9(3)
O(1)-C(10)-C(11)-C(12)	178.3(2)
C(9)-C(10)-C(11)-C(12)	-0.9(3)
O(1)-C(10)-C(11)-C(13)	-1.6(3)
C(9)-C(10)-C(11)-C(13)	179.3(2)
C(8)-C(7)-C(12)-C(11)	0.7(3)
N(2)-C(7)-C(12)-C(11)	-177.39(18)
C(10)-C(11)-C(12)-C(7)	0.1(3)
C(13)-C(11)-C(12)-C(7)	179.95(19)
C(14)-N(3)-C(13)-C(11)	-179.25(18)
C(12)-C(11)-C(13)-N(3)	-179.82(19)
C(10)-C(11)-C(13)-N(3)	0.0(3)
C(13)-N(3)-C(14)-C(19)	-171.4(2)
C(13)-N(3)-C(14)-C(15)	10.6(3)
C(19)-C(14)-C(15)-C(16)	1.7(3)
N(3)-C(14)-C(15)-C(16)	179.8(2)
C(14)-C(15)-C(16)-C(17)	0.0(3)
C(15)-C(16)-C(17)-C(18)	-1.3(3)

C(15)-C(16)-C(17)-C(20)	179.1(2)
C(16)-C(17)-C(18)-C(19)	1.0(3)
C(20)-C(17)-C(18)-C(19)	-179.5(2)
C(17)-C(18)-C(19)-C(14)	0.8(4)
C(15)-C(14)-C(19)-C(18)	-2.1(3)
N(3)-C(14)-C(19)-C(18)	179.7(2)

Table S9.

Bond lengths [Å] and angles [°] for **9**.

Ru(1)-O(1)	2.0594(14)	C(3)-H(3)	0.9300
Ru(1)-N(3)	2.0948(17)	C(4)-C(5)	1.385(3)
Ru(1)-C(25)	2.165(2)	C(4)-H(4)	0.9300
Ru(1)-C(26)	2.171(2)	C(5)-C(6)	1.388(3)
Ru(1)-C(22)	2.182(2)	C(5)-H(5)	0.9300
Ru(1)-C(24)	2.183(2)	C(7)-C(12)	1.378(3)
Ru(1)-C(23)	2.184(2)	C(7)-C(8)	1.410(3)
Ru(1)-C(21)	2.214(2)	C(8)-C(9)	1.365(3)
Ru(1)-Cl(1)	2.4264(6)	C(8)-H(8)	0.9300
N(3)-C(13)	1.292(3)	C(9)-C(10)	1.425(3)
N(3)-C(14)	1.438(2)	C(9)-H(9)	0.9300
O(1)-C(10)	1.296(2)	C(10)-C(11)	1.423(3)
C(21)-C(26)	1.406(3)	C(11)-C(12)	1.406(3)
C(21)-C(22)	1.420(4)	C(11)-C(13)	1.430(3)
C(21)-C(27)	1.501(4)	C(12)-H(12)	0.9300
C(22)-C(23)	1.397(3)	C(13)-H(13)	0.9300
C(22)-H(22)	0.9300	C(14)-C(15)	1.376(3)
C(23)-C(24)	1.425(3)	C(14)-C(19)	1.393(3)
C(23)-H(23)	0.9300	C(15)-C(16)	1.387(4)
C(24)-C(25)	1.407(3)	C(15)-H(15)	0.9300
C(24)-C(28)	1.510(3)	C(16)-C(17)	1.357(5)
C(25)-C(26)	1.421(3)	C(16)-H(16)	0.9300
C(25)-H(25)	0.9300	C(17)-C(18)	1.369(5)
C(26)-H(26)	0.9300	C(17)-H(17)	0.9300
C(1)-C(6)	1.382(3)	C(18)-C(19)	1.401(4)
C(1)-C(2)	1.390(3)	C(18)-H(18)	0.9300
C(1)-H(1)	0.9300	C(20)-H(20A)	0.9600
N(1)-N(2)	1.252(3)	C(20)-H(20B)	0.9600
N(1)-C(6)	1.431(3)	C(20)-H(20C)	0.9600
O(2)-C(19)	1.364(3)	C(27)-H(27A)	0.9600
O(2)-C(20)	1.418(4)	C(27)-H(27B)	0.9600
C(2)-C(3)	1.364(4)	C(27)-H(27C)	0.9600
C(2)-H(2)	0.9300	C(28)-C(29)	1.512(5)
N(2)-C(7)	1.415(3)	C(28)-C(30)	1.531(4)
C(3)-C(4)	1.378(4)	C(28)-H(28)	0.9800

C(29)-H(29A)	0.9600	C(30)-H(31A)	0.9600
C(29)-H(29B)	0.9600	C(30)-H(31B)	0.9600
C(29)-H(29C)	0.9600	C(30)-H(31C)	0.9600

O(1)-Ru(1)-N(3)	87.61(6)	C(23)-Ru(1)-Cl(1)	113.78(6)
O(1)-Ru(1)-C(25)	114.82(8)	C(21)-Ru(1)-Cl(1)	91.66(6)
N(3)-Ru(1)-C(25)	95.99(8)	C(13)-N(3)-C(14)	116.16(17)
O(1)-Ru(1)-C(26)	153.07(8)	C(13)-N(3)-Ru(1)	126.27(13)
N(3)-Ru(1)-C(26)	93.71(8)	C(14)-N(3)-Ru(1)	117.55(13)
C(25)-Ru(1)-C(26)	38.27(9)	C(10)-O(1)-Ru(1)	129.20(13)
O(1)-Ru(1)-C(22)	117.52(8)	C(26)-C(21)-C(22)	117.3(2)
N(3)-Ru(1)-C(22)	153.92(8)	C(26)-C(21)-C(27)	121.3(3)
C(25)-Ru(1)-C(22)	80.26(9)	C(22)-C(21)-C(27)	121.4(3)
C(26)-Ru(1)-C(22)	67.32(9)	C(26)-C(21)-Ru(1)	69.64(12)
O(1)-Ru(1)-C(24)	87.96(7)	C(22)-C(21)-Ru(1)	69.96(12)
N(3)-Ru(1)-C(24)	122.73(8)	C(27)-C(21)-Ru(1)	128.98(17)
C(25)-Ru(1)-C(24)	37.77(9)	C(23)-C(22)-C(21)	121.6(2)
C(26)-Ru(1)-C(24)	68.74(9)	C(23)-C(22)-Ru(1)	71.42(12)
C(22)-Ru(1)-C(24)	68.48(9)	C(21)-C(22)-Ru(1)	72.36(12)
O(1)-Ru(1)-C(23)	90.07(7)	C(23)-C(22)-H(22)	119.2
N(3)-Ru(1)-C(23)	160.78(8)	C(21)-C(22)-H(22)	119.2
C(25)-Ru(1)-C(23)	67.78(9)	Ru(1)-C(22)-H(22)	129.6
C(26)-Ru(1)-C(23)	79.92(9)	C(22)-C(23)-C(24)	121.0(2)
C(22)-Ru(1)-C(23)	37.32(9)	C(22)-C(23)-Ru(1)	71.26(13)
C(24)-Ru(1)-C(23)	38.08(9)	C(24)-C(23)-Ru(1)	70.91(12)
O(1)-Ru(1)-C(21)	155.19(8)	C(22)-C(23)-H(23)	119.5
N(3)-Ru(1)-C(21)	116.94(8)	C(24)-C(23)-H(23)	119.5
C(25)-Ru(1)-C(21)	68.62(9)	Ru(1)-C(23)-H(23)	131.2
C(26)-Ru(1)-C(21)	37.40(9)	C(25)-C(24)-C(23)	117.8(2)
C(22)-Ru(1)-C(21)	37.67(9)	C(25)-C(24)-C(28)	123.1(2)
C(24)-Ru(1)-C(21)	81.70(8)	C(23)-C(24)-C(28)	119.1(2)
C(23)-Ru(1)-C(21)	67.99(9)	C(25)-C(24)-Ru(1)	70.44(12)
O(1)-Ru(1)-Cl(1)	86.67(4)	C(23)-C(24)-Ru(1)	71.01(12)
N(3)-Ru(1)-Cl(1)	85.14(5)	C(28)-C(24)-Ru(1)	127.85(16)
C(25)-Ru(1)-Cl(1)	158.50(7)	C(24)-C(25)-C(26)	120.6(2)
C(26)-Ru(1)-Cl(1)	120.25(7)	C(24)-C(25)-Ru(1)	71.79(12)
C(22)-Ru(1)-Cl(1)	89.30(6)	C(26)-C(25)-Ru(1)	71.07(12)
C(24)-Ru(1)-Cl(1)	151.35(6)	C(24)-C(25)-H(25)	119.7

C(26)-C(25)-H(25)	119.7	O(1)-C(10)-C(11)	124.85(17)
Ru(1)-C(25)-H(25)	130.0	O(1)-C(10)-C(9)	117.77(17)
C(21)-C(26)-C(25)	121.6(2)	C(11)-C(10)-C(9)	117.38(17)
C(21)-C(26)-Ru(1)	72.95(12)	C(12)-C(11)-C(10)	119.29(18)
C(25)-C(26)-Ru(1)	70.66(12)	C(12)-C(11)-C(13)	116.98(18)
C(21)-C(26)-H(26)	119.2	C(10)-C(11)-C(13)	123.67(17)
C(25)-C(26)-H(26)	119.2	C(7)-C(12)-C(11)	121.96(19)
Ru(1)-C(26)-H(26)	129.8	C(7)-C(12)-H(12)	119.0
C(6)-C(1)-C(2)	120.0(3)	C(11)-C(12)-H(12)	119.0
C(6)-C(1)-H(1)	120.0	N(3)-C(13)-C(11)	127.24(18)
C(2)-C(1)-H(1)	120.0	N(3)-C(13)-H(13)	116.4
N(2)-N(1)-C(6)	113.53(18)	C(11)-C(13)-H(13)	116.4
C(19)-O(2)-C(20)	118.3(3)	C(15)-C(14)-C(19)	120.6(2)
C(3)-C(2)-C(1)	120.2(3)	C(15)-C(14)-N(3)	119.4(2)
C(3)-C(2)-H(2)	119.9	C(19)-C(14)-N(3)	119.9(2)
C(1)-C(2)-H(2)	119.9	C(14)-C(15)-C(16)	119.8(3)
N(1)-N(2)-C(7)	115.19(18)	C(14)-C(15)-H(15)	120.1
C(2)-C(3)-C(4)	120.1(2)	C(16)-C(15)-H(15)	120.1
C(2)-C(3)-H(3)	119.9	C(17)-C(16)-C(15)	119.8(3)
C(4)-C(3)-H(3)	119.9	C(17)-C(16)-H(16)	120.1
C(3)-C(4)-C(5)	120.5(3)	C(15)-C(16)-H(16)	120.1
C(3)-C(4)-H(4)	119.7	C(16)-C(17)-C(18)	121.4(3)
C(5)-C(4)-H(4)	119.7	C(16)-C(17)-H(17)	119.3
C(4)-C(5)-C(6)	119.4(2)	C(18)-C(17)-H(17)	119.3
C(4)-C(5)-H(5)	120.3	C(17)-C(18)-C(19)	120.0(3)
C(6)-C(5)-H(5)	120.3	C(17)-C(18)-H(18)	120.0
C(1)-C(6)-C(5)	119.8(2)	C(19)-C(18)-H(18)	120.0
C(1)-C(6)-N(1)	116.3(2)	O(2)-C(19)-C(14)	115.7(2)
C(5)-C(6)-N(1)	123.8(2)	O(2)-C(19)-C(18)	125.8(3)
C(12)-C(7)-C(8)	118.91(18)	C(14)-C(19)-C(18)	118.4(3)
C(12)-C(7)-N(2)	115.55(19)	O(2)-C(20)-H(20A)	109.5
C(8)-C(7)-N(2)	125.53(19)	O(2)-C(20)-H(20B)	109.5
C(9)-C(8)-C(7)	120.41(19)	H(20A)-C(20)-H(20B)	109.5
C(9)-C(8)-H(8)	119.8	O(2)-C(20)-H(20C)	109.5
C(7)-C(8)-H(8)	119.8	H(20A)-C(20)-H(20C)	109.5
C(8)-C(9)-C(10)	121.96(19)	H(20B)-C(20)-H(20C)	109.5
C(8)-C(9)-H(9)	119.0	C(21)-C(27)-H(27A)	109.5
C(10)-C(9)-H(9)	119.0	C(21)-C(27)-H(27B)	109.5

H(27A)-C(27)-H(27B)	109.5
C(21)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(24)-C(28)-C(29)	113.9(3)
C(24)-C(28)-C(30)	109.3(2)
C(29)-C(28)-C(30)	111.6(3)
C(24)-C(28)-H(28)	107.2
C(29)-C(28)-H(28)	107.2
C(30)-C(28)-H(28)	107.2
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(31A)	109.5
C(28)-C(30)-H(31B)	109.5
H(31A)-C(30)-H(31B)	109.5
C(28)-C(30)-H(31C)	109.5
H(31A)-C(30)-H(31C)	109.5
H(31B)-C(30)-H(31C)	109.5

Table S10.

Torsion angles [°] for **9**.

C(26)-C(21)-C(22)-C(23)	-1.1(3)
C(27)-C(21)-C(22)-C(23)	-178.1(2)
Ru(1)-C(21)-C(22)-C(23)	-53.95(18)
C(26)-C(21)-C(22)-Ru(1)	52.82(17)
C(27)-C(21)-C(22)-Ru(1)	-124.2(2)
C(21)-C(22)-C(23)-C(24)	1.7(3)
Ru(1)-C(22)-C(23)-C(24)	-52.63(18)
C(21)-C(22)-C(23)-Ru(1)	54.37(18)
C(22)-C(23)-C(24)-C(25)	-1.6(3)
Ru(1)-C(23)-C(24)-C(25)	-54.41(17)
C(22)-C(23)-C(24)-C(28)	176.2(2)
Ru(1)-C(23)-C(24)-C(28)	123.5(2)
C(22)-C(23)-C(24)-Ru(1)	52.79(18)
C(23)-C(24)-C(25)-C(26)	1.0(3)
C(28)-C(24)-C(25)-C(26)	-176.8(2)
Ru(1)-C(24)-C(25)-C(26)	-53.72(18)
C(23)-C(24)-C(25)-Ru(1)	54.69(17)
C(28)-C(24)-C(25)-Ru(1)	-123.1(2)
C(22)-C(21)-C(26)-C(25)	0.5(3)
C(27)-C(21)-C(26)-C(25)	177.5(2)
Ru(1)-C(21)-C(26)-C(25)	53.45(18)
C(22)-C(21)-C(26)-Ru(1)	-52.97(17)
C(27)-C(21)-C(26)-Ru(1)	124.0(2)
C(24)-C(25)-C(26)-C(21)	-0.4(3)
Ru(1)-C(25)-C(26)-C(21)	-54.49(19)
C(24)-C(25)-C(26)-Ru(1)	54.05(18)
C(6)-C(1)-C(2)-C(3)	0.9(4)
C(6)-N(1)-N(2)-C(7)	-177.95(18)
C(1)-C(2)-C(3)-C(4)	-0.1(4)
C(2)-C(3)-C(4)-C(5)	-0.3(4)
C(3)-C(4)-C(5)-C(6)	0.0(4)
C(2)-C(1)-C(6)-C(5)	-1.2(4)
C(2)-C(1)-C(6)-N(1)	-179.2(2)
C(4)-C(5)-C(6)-C(1)	0.8(4)
C(4)-C(5)-C(6)-N(1)	178.6(2)

N(2)-N(1)-C(6)-C(1)	-171.9(2)
N(2)-N(1)-C(6)-C(5)	10.2(3)
N(1)-N(2)-C(7)-C(12)	171.5(2)
N(1)-N(2)-C(7)-C(8)	-7.4(3)
C(12)-C(7)-C(8)-C(9)	-1.3(3)
N(2)-C(7)-C(8)-C(9)	177.5(2)
C(7)-C(8)-C(9)-C(10)	-1.4(3)
Ru(1)-O(1)-C(10)-C(11)	-7.2(3)
Ru(1)-O(1)-C(10)-C(9)	173.22(14)
C(8)-C(9)-C(10)-O(1)	-177.61(19)
C(8)-C(9)-C(10)-C(11)	2.7(3)
O(1)-C(10)-C(11)-C(12)	179.04(19)
C(9)-C(10)-C(11)-C(12)	-1.3(3)
O(1)-C(10)-C(11)-C(13)	-4.0(3)
C(9)-C(10)-C(11)-C(13)	175.58(19)
C(8)-C(7)-C(12)-C(11)	2.7(3)
N(2)-C(7)-C(12)-C(11)	-176.2(2)
C(10)-C(11)-C(12)-C(7)	-1.4(3)
C(13)-C(11)-C(12)-C(7)	-178.5(2)
C(14)-N(3)-C(13)-C(11)	-177.4(2)
Ru(1)-N(3)-C(13)-C(11)	1.0(3)
C(12)-C(11)-C(13)-N(3)	-175.8(2)
C(10)-C(11)-C(13)-N(3)	7.2(3)
C(13)-N(3)-C(14)-C(15)	-106.6(3)
Ru(1)-N(3)-C(14)-C(15)	74.9(2)
C(13)-N(3)-C(14)-C(19)	77.3(3)
Ru(1)-N(3)-C(14)-C(19)	-101.2(2)
C(19)-C(14)-C(15)-C(16)	1.1(4)
N(3)-C(14)-C(15)-C(16)	-174.9(3)
C(14)-C(15)-C(16)-C(17)	0.4(5)
C(15)-C(16)-C(17)-C(18)	-1.3(6)
C(16)-C(17)-C(18)-C(19)	0.8(6)
C(20)-O(2)-C(19)-C(14)	-172.2(3)
C(20)-O(2)-C(19)-C(18)	9.9(5)
C(15)-C(14)-C(19)-O(2)	-179.6(2)
N(3)-C(14)-C(19)-O(2)	-3.6(3)
C(15)-C(14)-C(19)-C(18)	-1.6(4)
N(3)-C(14)-C(19)-C(18)	174.4(2)

C(17)-C(18)-C(19)-O(2)	178.4(3)
C(17)-C(18)-C(19)-C(14)	0.6(5)
C(25)-C(24)-C(28)-C(29)	28.5(4)
C(23)-C(24)-C(28)-C(29)	-149.3(3)
Ru(1)-C(24)-C(28)-C(29)	-61.5(3)
C(25)-C(24)-C(28)-C(30)	-97.1(3)
C(23)-C(24)-C(28)-C(30)	85.2(3)
Ru(1)-C(24)-C(28)-C(30)	172.9(2)

Table S11.

Hydrogen bonds for **9** [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8)...Cl(1)#1	0.93	2.96	3.654(2)	132.2
C(3)-H(3)...Cl(1)#2	0.93	2.73	3.649(2)	171.3

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z+1 #2 -x,-y+2,-z+1