Supporting information

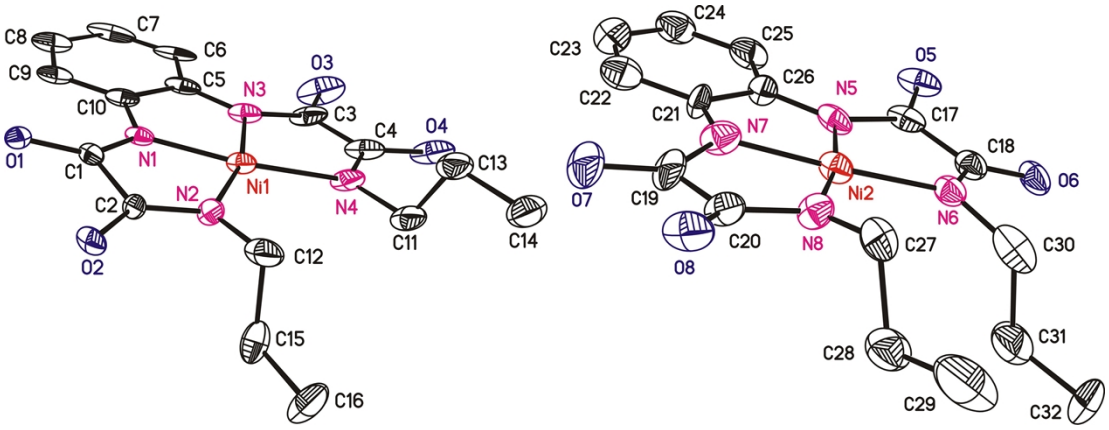

Figure S1 ORTEP diagram (25 % ellipsoid probability) of the molecular structures of **6A** (left) and **6B** (right). All hydrogen atoms are omitted for clarity.

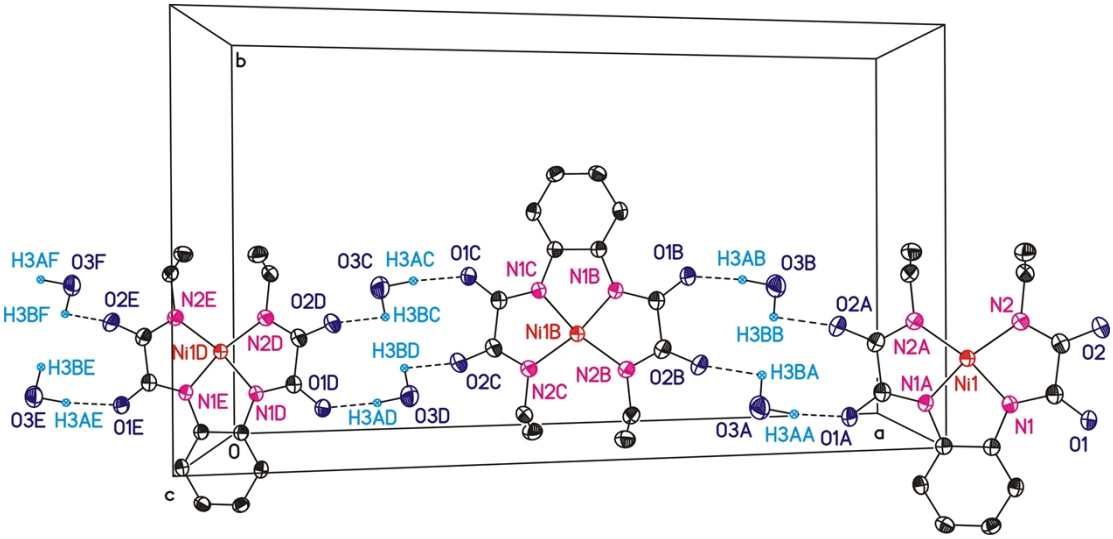

Figure S2 Graphical illustration of a selected part of one 1D chain formed by **5'** in the solid state due to formation of intermolecular hydrogen bonds. All $[^{n}Bu_4N]^+$ cations and *C*-bonded hydrogen atoms are omitted for clarity. Label "A" to "F" refers to atoms of a 1st to the 6th symmetry generated asymmetric unit of **5'**.

Table S1 Selected bond lengths (Å) and angles (°) of the intermolecular hydrogen bonds of **5'**.

D–H···A	D···A	D–H···A
O3–H3A···O1	2.833	133
O3–H3B···O2^{i}	2.974	109

Symmetry code: (i) ½ – x, ½ – y, 1 – z.

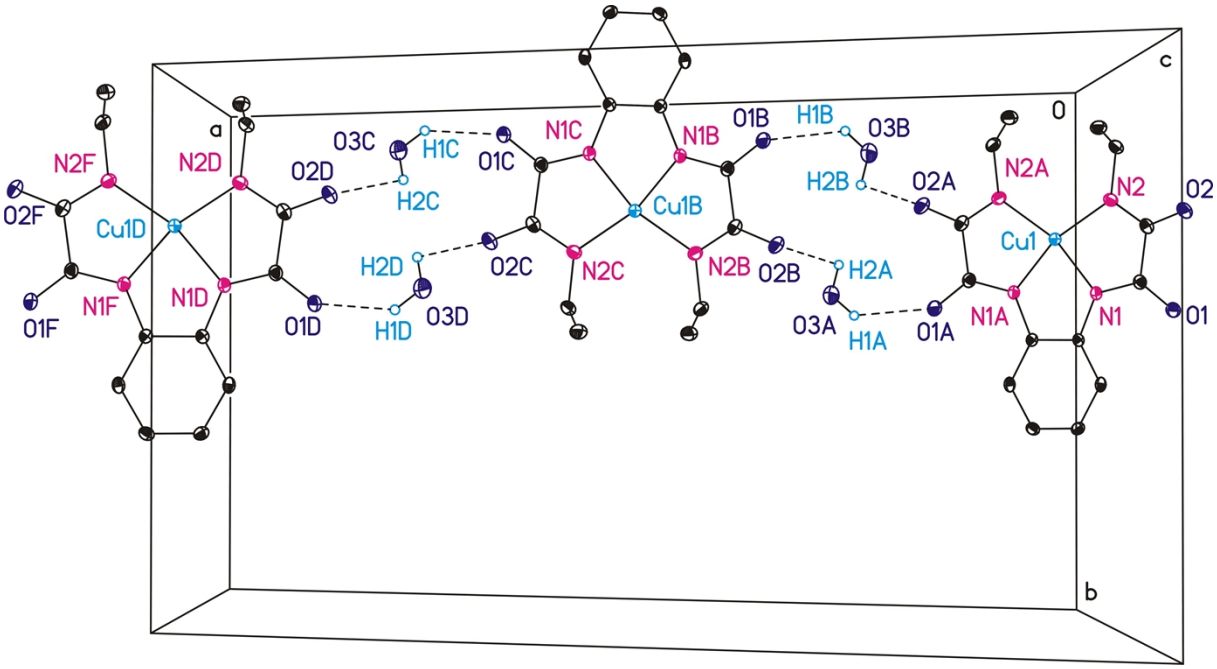

Figure S3 Graphical illustration of a selected part of one 1D chain formed by **8'** in the solid state due to formation of intermolecular hydrogen bonds. All $[^{n}Bu_4N]^+$ cations and *C*-bonded hydrogen atoms are omitted for clarity. Label "A" to "F" refers to atoms of a 1st to the 6th symmetry generated asymmetric unit of **8'**.

Table S2 Selected bond lengths (Å) and angles (°) of the intermolecular hydrogen bonds of **8'**.

D–H···A	D···A	D–H···A
O3–H1···O1	2.832	119
O3–H2···O2^{i}	2.992	135

Symmetry codes: (i) ½ – x, ½ – y, 1 – z.

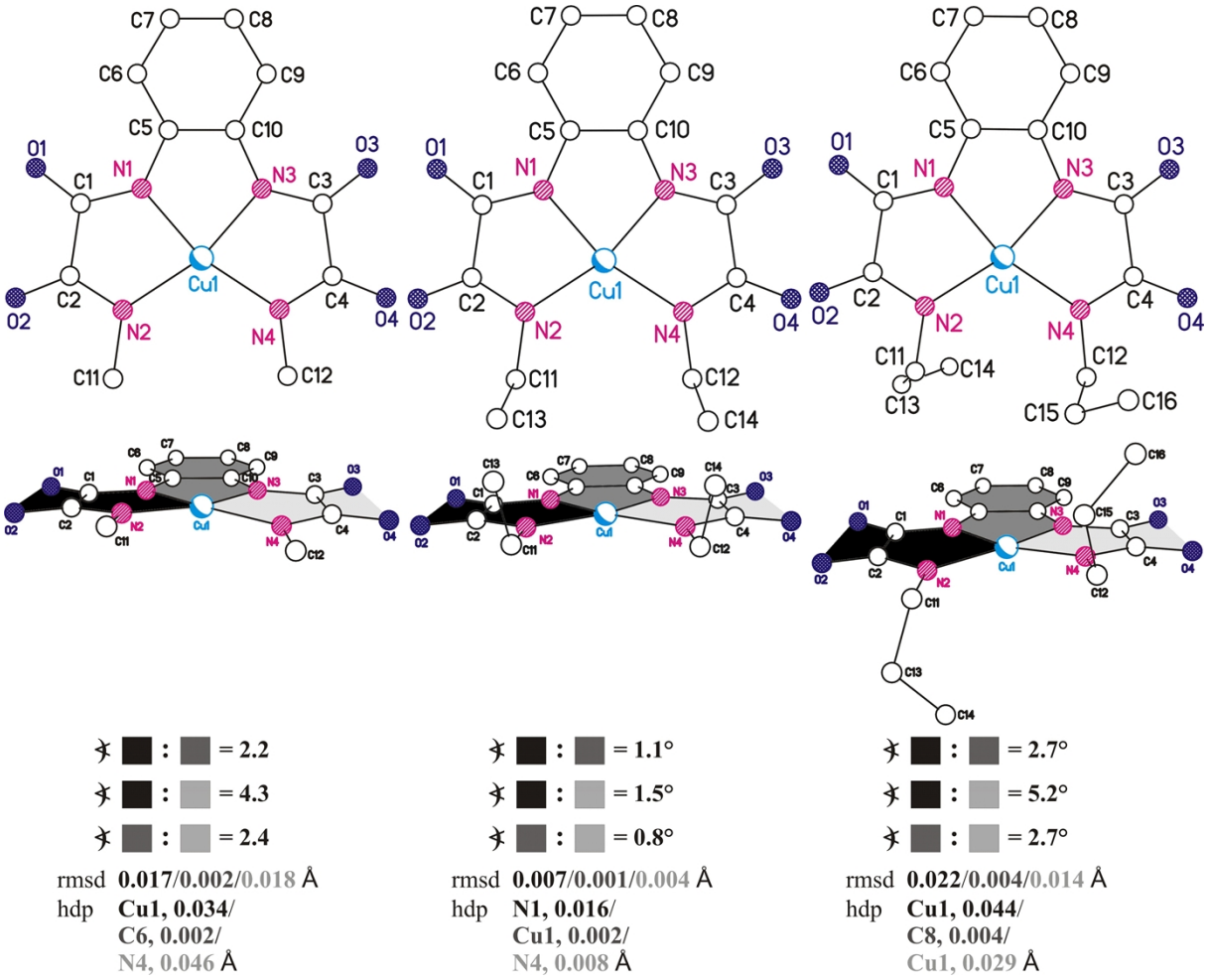

Figure S4 Ball-and-stick models of the molecular structures of **7A**^{calc}, **8A**^{calc} and **9A**^{calc} (left to right). Above: Top view. Below: Side view. All hydrogen atoms are omitted for clarity. The sign ∢ refers to the interplanar angles.

Table S3 Selected bond lengths (Å) and angles (°) of **7A–9A** and of the quantum chemically calculated related $[Cu(opboR_2]^{2-}$ fragments denoted as **7A**^{calc}**–9A**^{calc}

	7A	**7A**^{calc}	**8A**^{a}	**8A**^{calc}	**9A**	**9A**^{calc}
			Bond lengths			
N1–Cu1	1.938(16)	1.970	1.9372(17)	1.974	1.934(6)	1.971
N2–Cu1	1.952(17)	2.001	1.9643(18)	2.011	1.967(7)	2.012
N3–Cu1	1.938(17)	1.971	1.9372(17)	1.973	1.936(7)	1.971
N4–Cu1	1.953(17)	2.001	1.9643(18)	2.009	1.942(7)	2.009
C1–O1	1.239(2)	1.235	1.244(3)	1.234	1.244(3)	1.234
C2–O2	1.251(2)	1.240	1.258(3)	1.240	1.240(7)	1.239
C3–O3	1.243(2)	1.235	1.244(3)	1.234	1.171(8)	1.234
C4–O4	1.250(3)	1.240	1.258(3)	1.240	1.312(10)	1.239
C1–C2	1.545(3)	1.564	1.551(3)	1.562	1.561(11)	1.563
C3–C4	1.548(3)	1.564	1.551(3)	1.563	1.559(14)	1.565
			Bond angles			
N1–Cu1–N3	82.20(7)	81.81	81.95(10)	81.65	80.8(3)	81.70
N2–Cu1–N4	111.18(7)	113.72	112.37(11)	113.96	111.9(3)	113.88
N1–Cu1–N2	83.30(7)	82.38	83.05(7)	82.18	83.2(3)	82.30
N3–Cu1–N4	83.50(7)	82.29	83.05(7)	82.22	84.2(3)	82.31
N1–Cu1–N4	165.23(7)	163.59	164.03(7)	163.83	164.9(3)	163.60
N2–Cu1–N3	165.05(7)	163.76	164.03(7)	163.82	163.9(3)	163.55
O1–C1–N1	128.7(2)	128.19	128.4(2)	128.20	128.2(10)	128.26
O1–C1–C2	120.50(18)	120.28	120.23(18)	120.21	121.1(6)	120.18
N1–C1–C2	110.79(18)	111.52	111.38(18)	111.60	110.7(7)	111.56
O2–C2–N2	126.2(2)	125.65	127.2(2)	125.91	127.6(9)	125.87
O2–C2–C1	118.68(19)	119.79	118.5(2)	119.41	117.4(7)	119.35
N2–C2–C1	115.10(18)	114.55	114.31(18)	114.68	115.0(6)	114.78
O3–C3–N3	128.3(2)	128.18	128.4(2)	128.22	132.8(13)	128.20
O3–C3–C4	120.31(19)	120.28	120.23(18)	120.18	117.7(10)	120.09
N3–C3–C4	111.42(18)	111.54	111.38(18)	111.59	109.4(7)	111.71
O4–C4–N4	126.3(2)	125.79	127.2(2)	125.94	122.1(13)	126.56
O4–C4–C3	119.0(2)	119.75	118.5(2)	119.43	122.0(8)	119.02
N4–C4–C3	114.74(18)	114.46	114.31(18)	114.63	115.9(8)	114.42

[b] For **8A** the labeling is as follows: N3 = N1A, C3 = C3A, O3 = O1A, N4 = N2A, C4 = C4A, O4 = O4A. Symmetry code "A": –x, y, –z + ½.

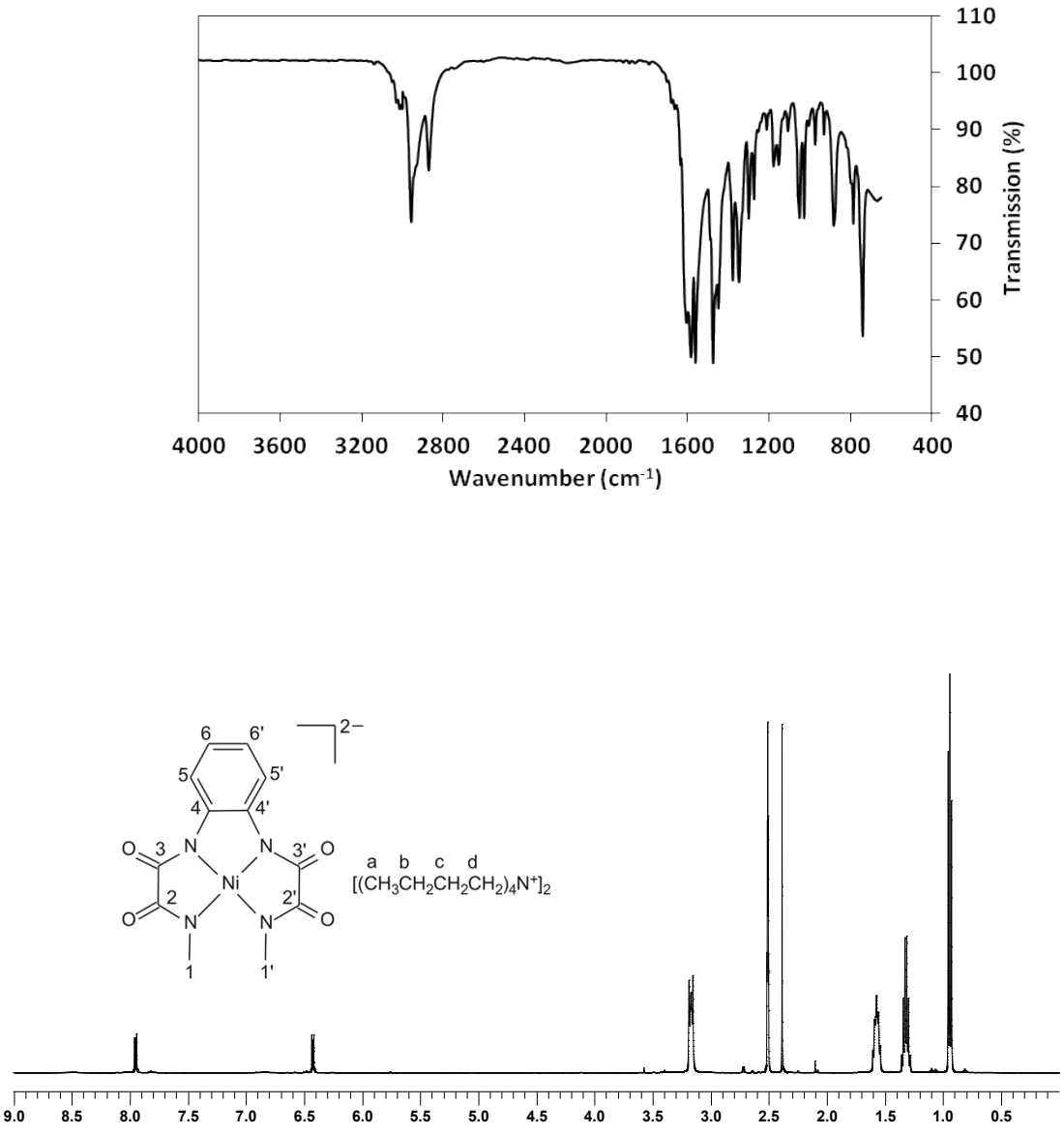

Figure S5 IR (above) and ^{1}H NMR (down) spectra of **4**

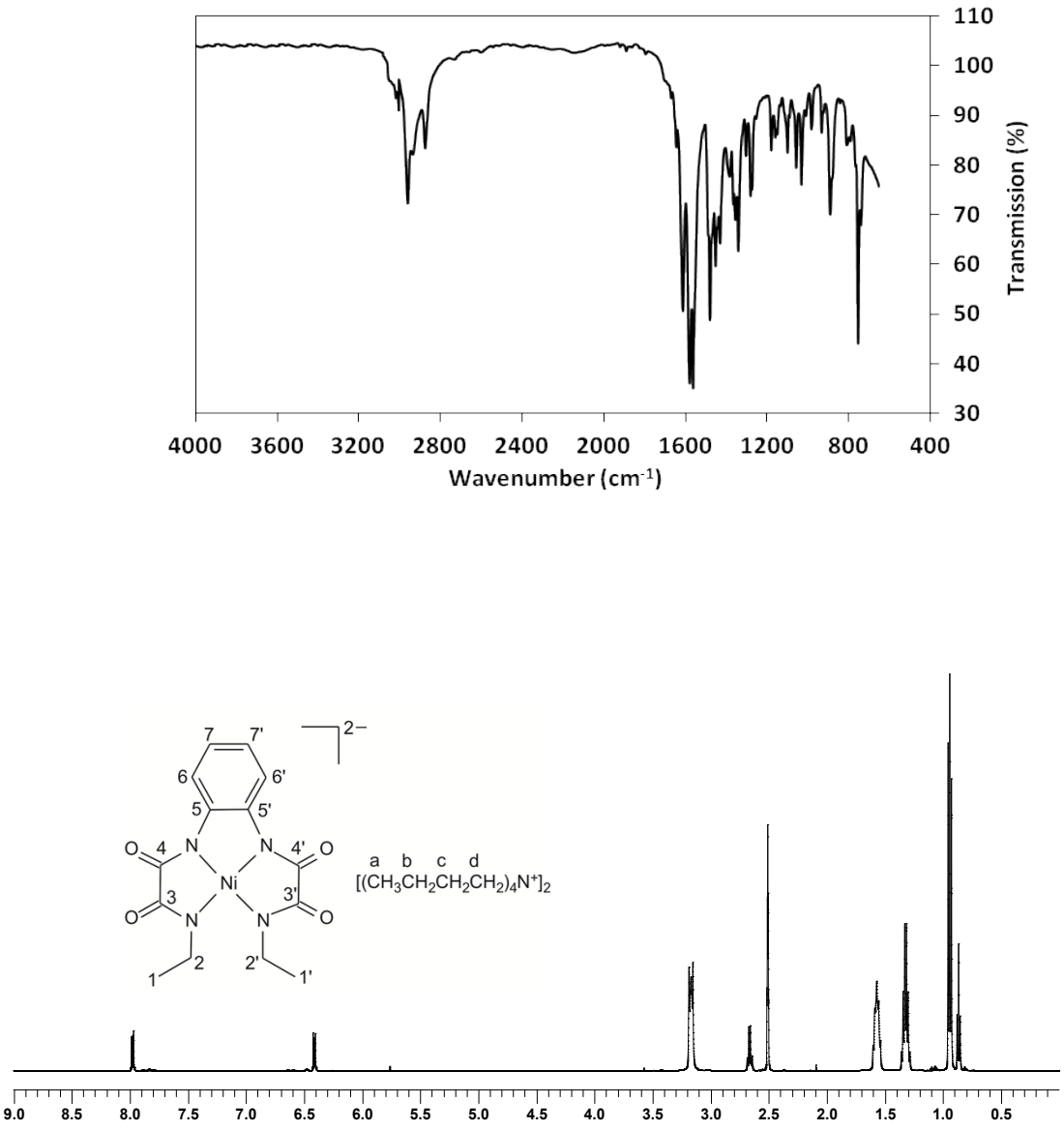

Figure S6 IR (above) and ^{1}H NMR (down) spectra of **5**

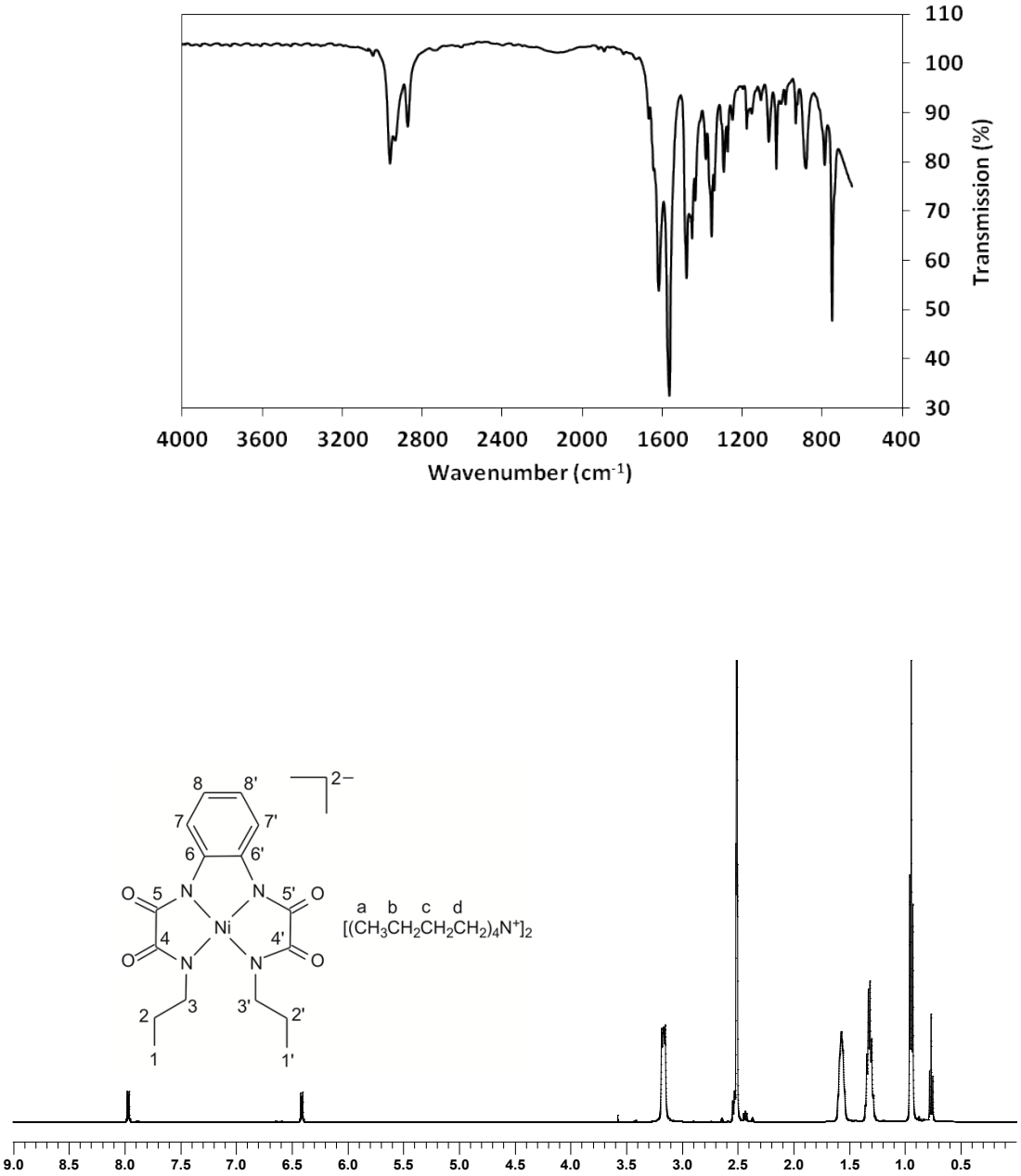

Figure S7 IR (above) and ^{1}H NMR (down) spectra of **6**

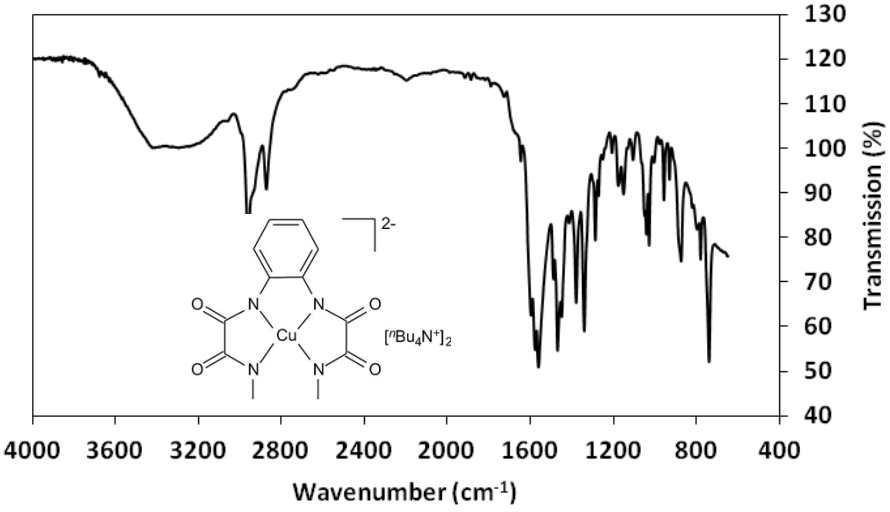

Figure S8 IR spectrum of **7**

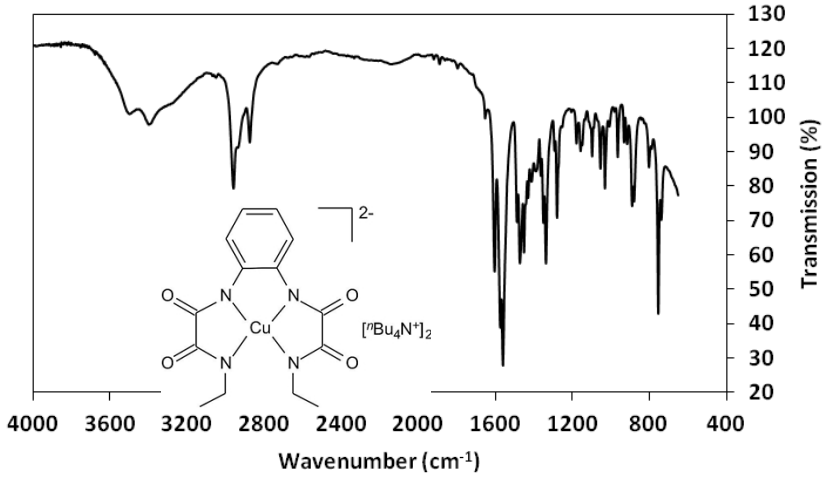

Figure S9 IR spectrum of **8**

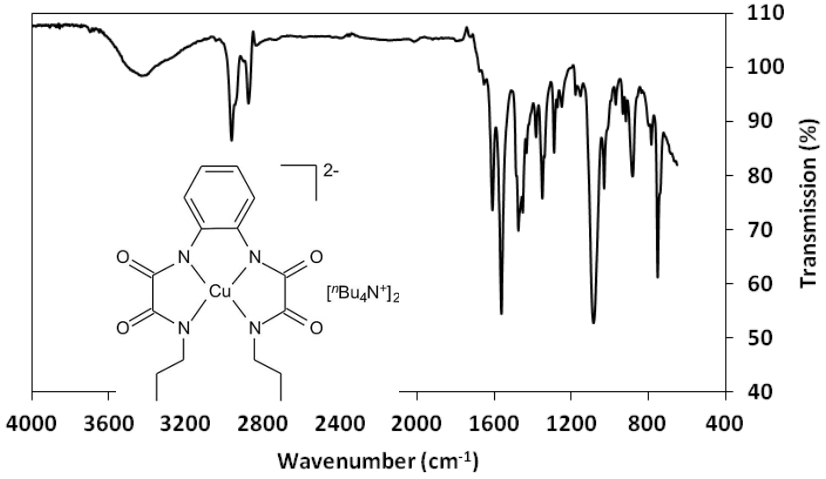

Figure S10 IR spectrum of **9**

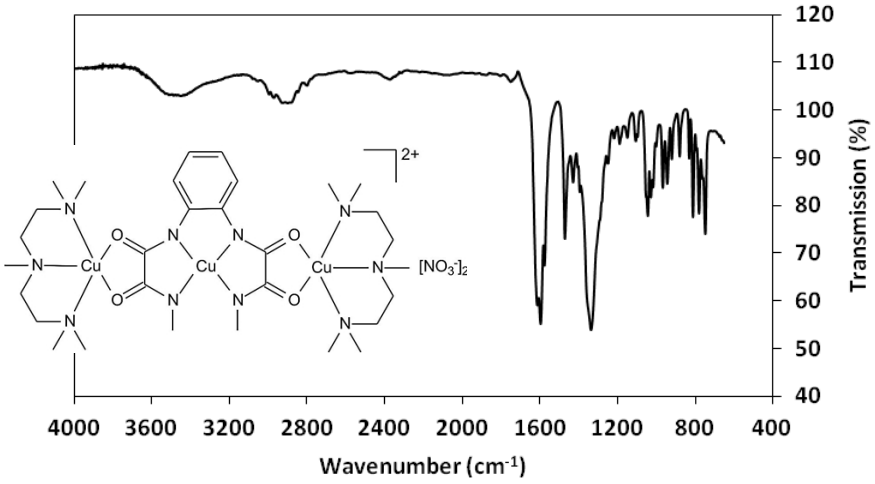

Figure S11 IR spectrum of **10**

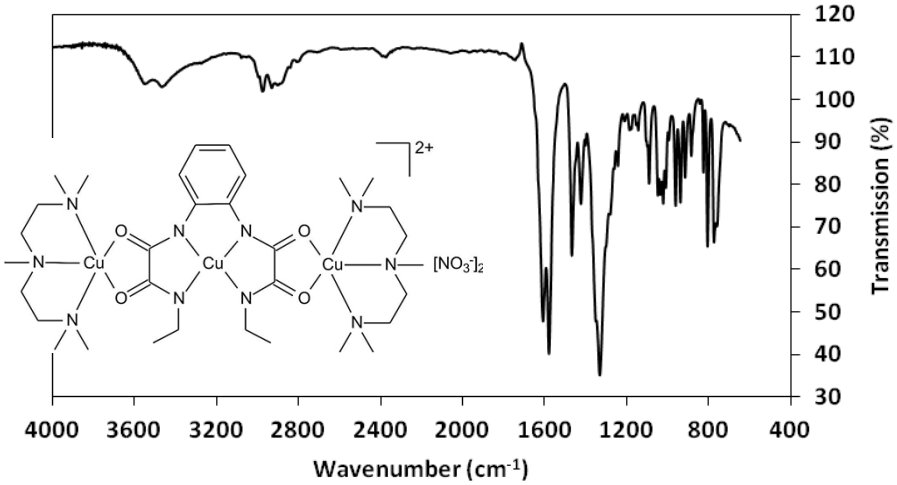

Figure S12 IR spectrum of **11**

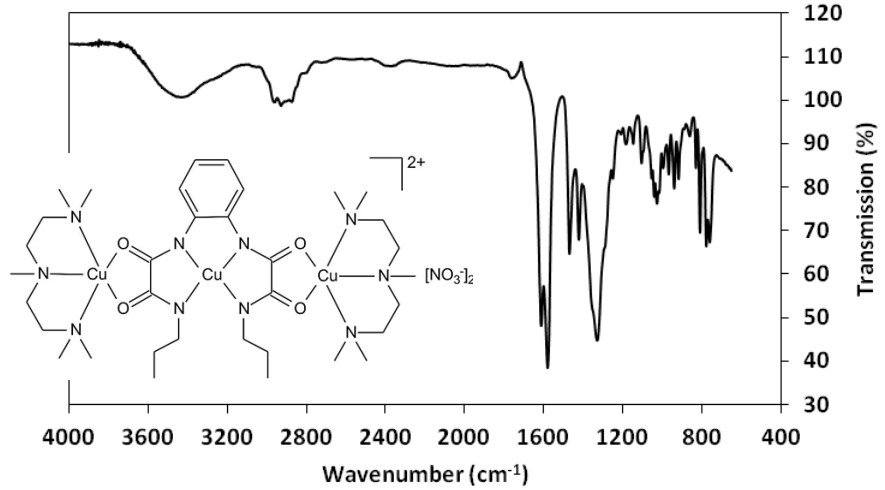

Figure S13 IR spectrum of **12**