Electronic Supplementary Material (ESI) for CrystEngComm

Bis(morpholine) hydrogen bond *pincer* – a novel series of heteroleptic Cu(II) coordination compounds as receptors for electron rich guests

Supplementary information

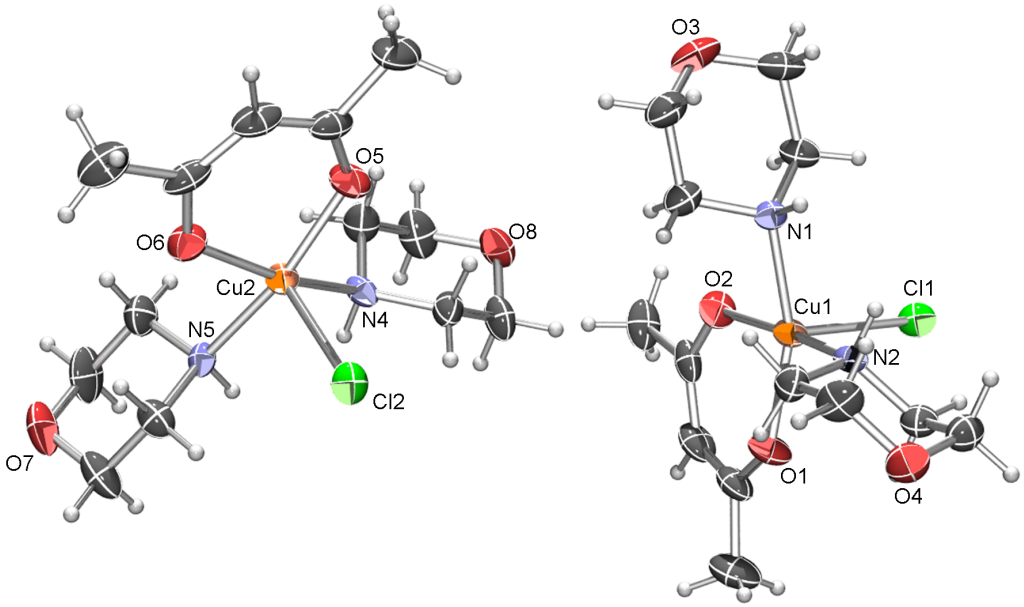


Figure S1. Ortep plot of the asymmetric unit in **I** with the labelling scheme for non-CH atoms. Thermal ellipsoids are shown for 50 % probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

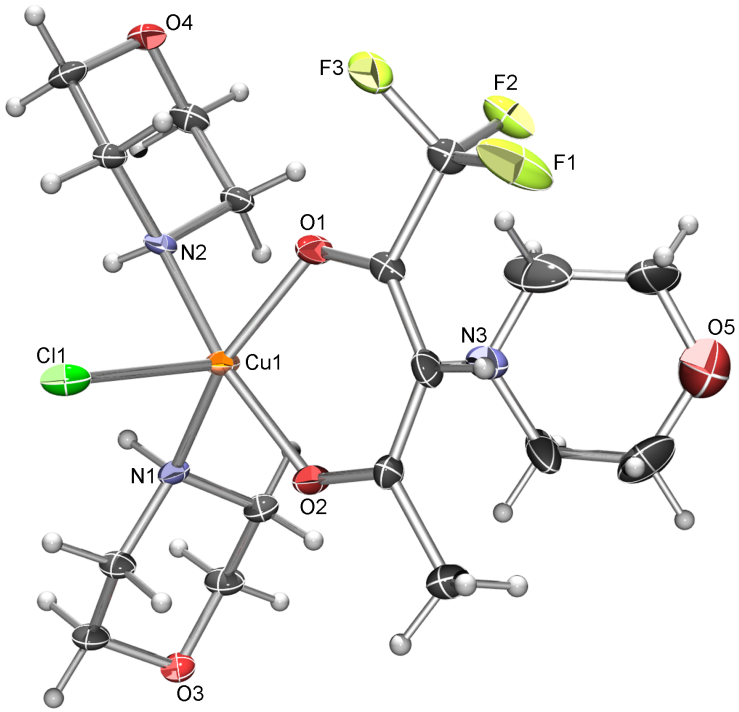


Figure 2. Ortep plot of the asymmetric unit in **II** with the labelling scheme for non-CH atoms. Thermal ellipsoids are shown for 50 % probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

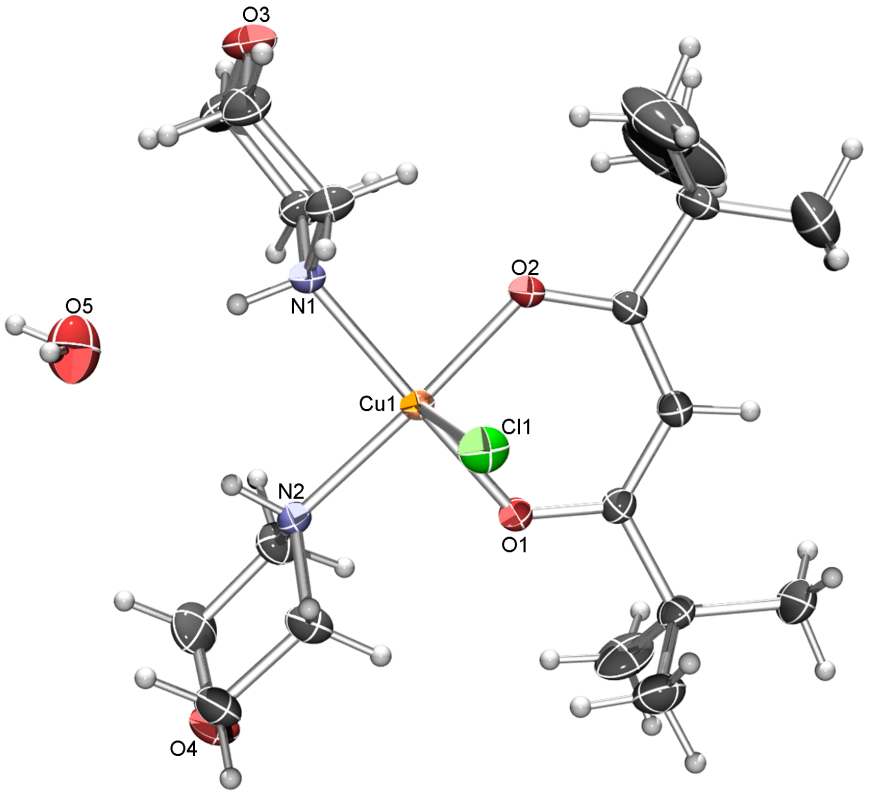


Figure S3. Ortep plot of the asymmetric unit in **III** with the labelling scheme for non-CH atoms. Thermal ellipsoids are shown for 50 % probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

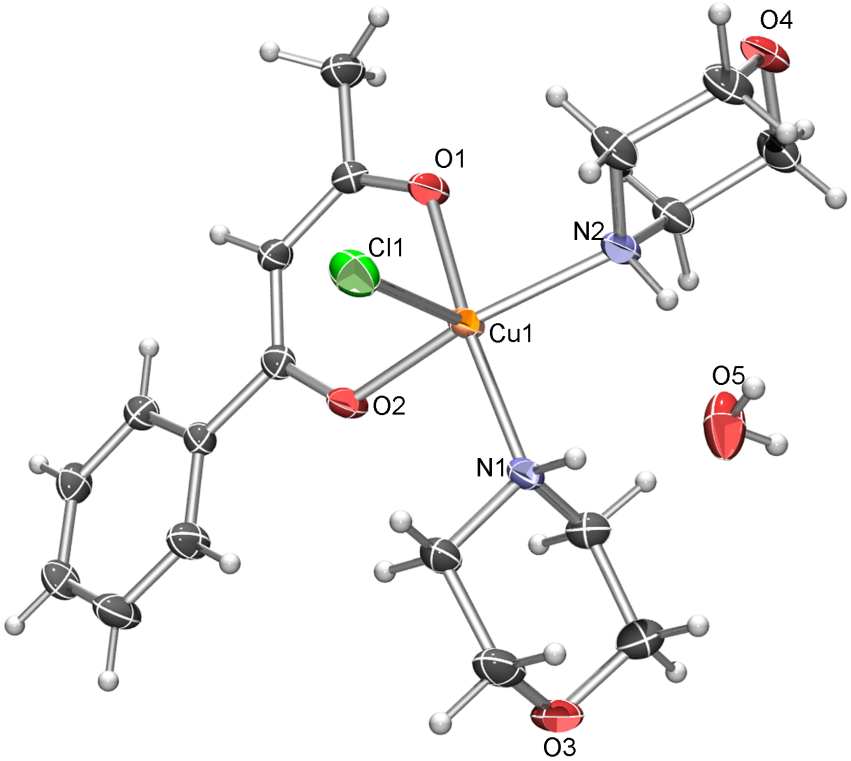


Figure S4. Ortep plot of the asymmetric unit in **IV** with the labelling scheme for non-CH atoms. Thermal ellipsoids are shown for 50 % probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

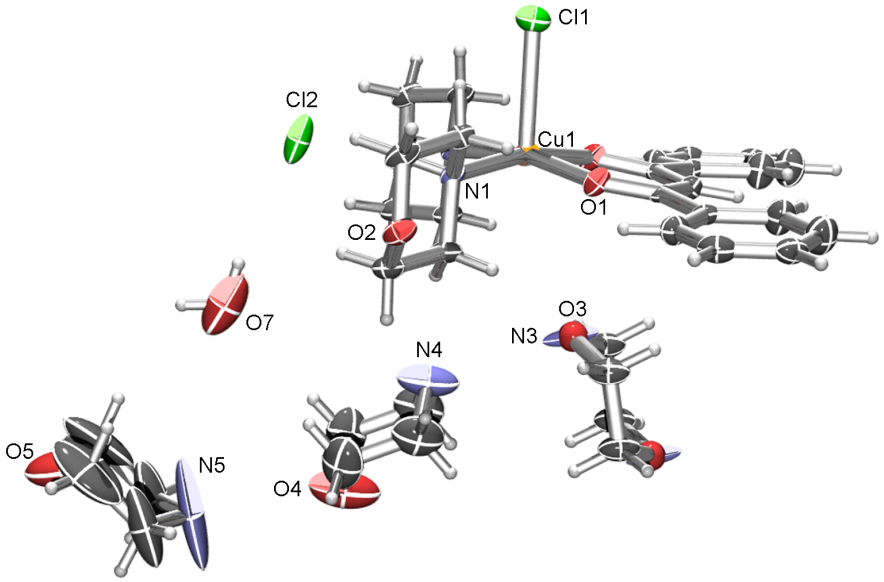


Figure S5. Ortep plot of a double asymmetric unit in **V** with the labelling scheme for non-CH atoms. Thermal ellipsoids are shown for 50 % probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

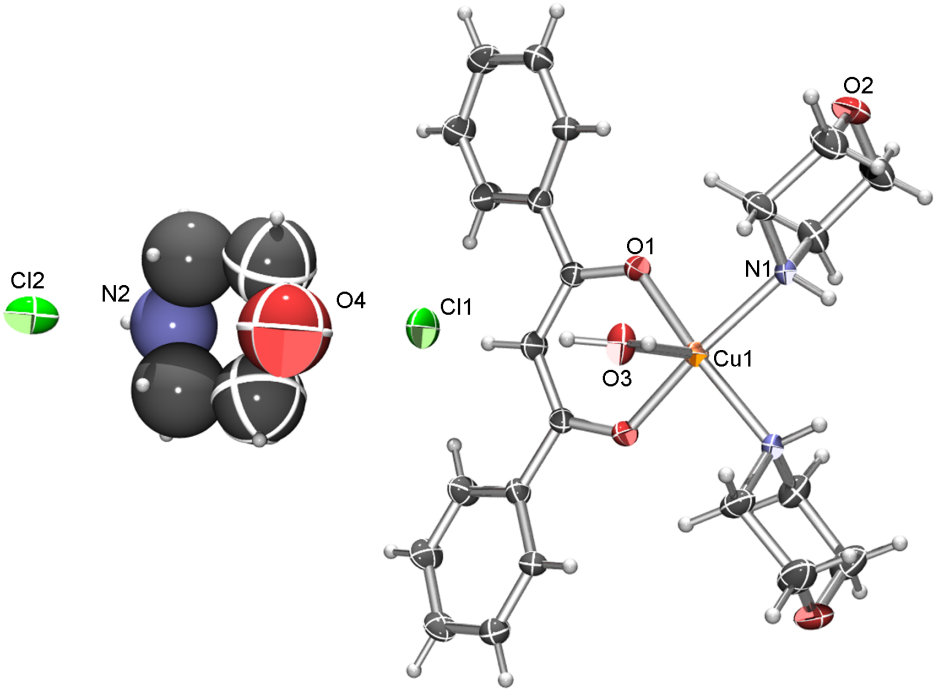


Figure S6. Ortep plot of a double asymmetric unit in **VI** with the labelling scheme for non-CH atoms. Thermal ellipsoids are shown for 50 % probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

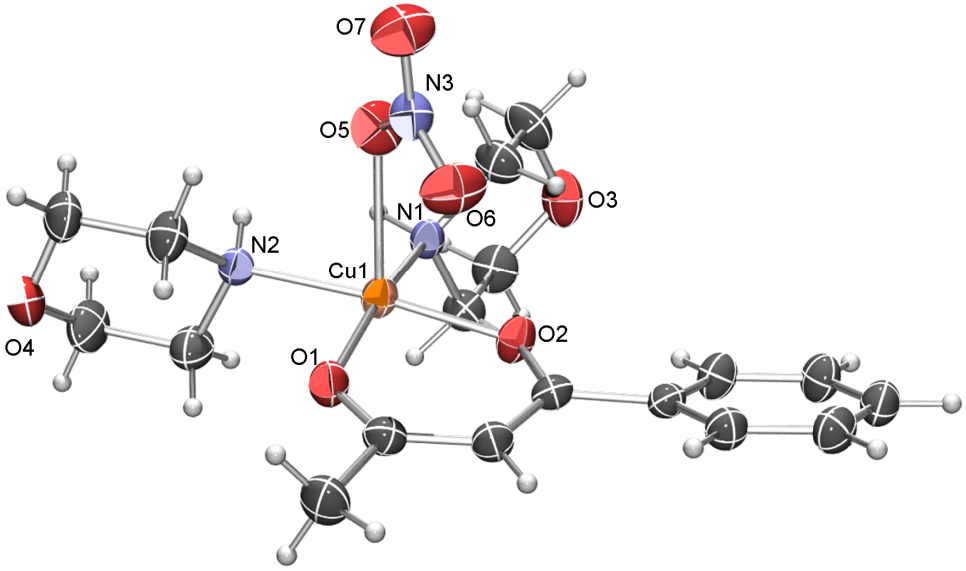


Figure S7. Ortep plot of the asymmetric unit in **VII** with the labelling scheme for non-CH atoms. Thermal ellipsoids are shown for 50 % probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

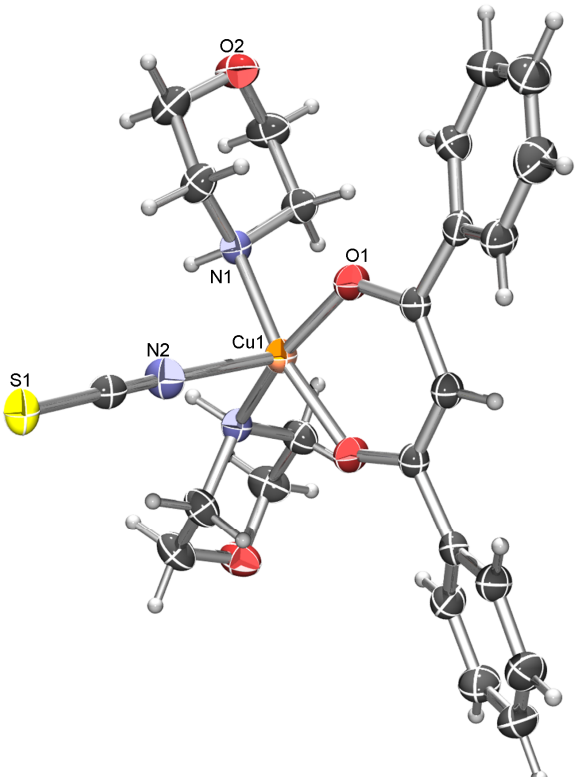


Figure S8. Ortep plot of a double asymmetric unit in **VIII** with the labelling scheme for non-CH atoms. Thermal ellipsoids are shown for 50 % probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

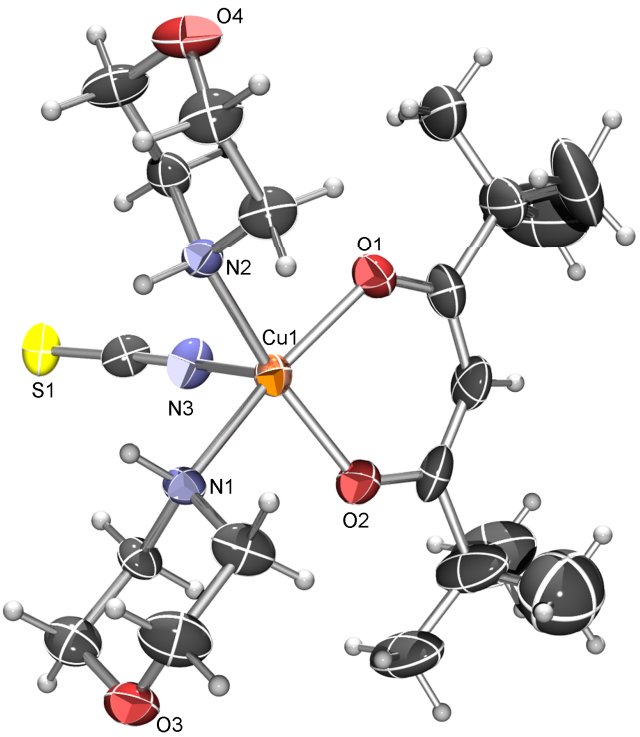


Figure S6. Ortep plot of the asymmetric unit in **IX** with the labelling scheme for non-CH atoms. Thermal ellipsoids are shown for 50 % probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

Table SI 1. Hydrogen bonding geometry in **I**.*

D–H···A[operator]	*d*(D–H)	*d*(D···A)	*d*(H···A)	*φ*(D–H···A)
C11–H11B···O7[a]	0.971	3.270(7)	2.467	139.9
N1–H1N···Cl1[b]	0.910(16)	3.255(7)	2.345(15)	177.6 (1.2)
N2–H2N···Cl1[b]	0.910(15)	3.347(7)	2.510(16)	153.1(1.2)
C20–H2OB···O4[c]	0.969	3.364(8)	2.549	141.7
N3–H3N···Cl2[d]	0.909(17)	3.283(7)	2.409(16)	161.2(1.3)
N4–H4N···Cl2[d]	0.911(16)	3.288(7)	2.382(15)	173.5(1.4)

a) –*x*+3/2, *y*+1/2, –*z*+3/2; b) –*x*+3/2, *y*+1/2, –*z*+1/2; c) *x*–1/2, –*y*+1/2, *z*+1/2; d) –*x*+3/2, *y*–1/2, –*z*+3/2

Table SI 2. Hydrogen bonding geometry in **II**.

D–H···A[operator]	*d*(D–H)	*d*(D···A)	*d*(H···A)	*φ*(D–H···A)
C10–H10B···O3[a]	0.970	3.297(7)	2.462	144.12
C9–H9A···O4[b]	0.970	3.458(7)	2.724	132.87
C16–H16B···O4[b]	0.971	3.426(6)	2.498	159.82
N2–H2N···Cl1[c]	0.80(10)	3.328(9)	2.61(10)	152(9)
N1–H1N···Cl1[c]	0.96(7)	3.248(8)	2.29(6)	171(5)

a) –*x*+3/2, –*y*, *z*–1/2; b) –*x*+3/2, –*y*, *z*+1/2; c) –*x*+1/2, –*y*+1/2, –*z*+1

Table SI 3. Hydrogen bonding geometry in **III**.

D–H···A[operator]	*d*(D–H)	*d*(D···A)	*d*(H···A)	*φ*(D–H···A)
O5–H1W···Cl2[a]	0.82(4)	3.486(5)	2.72 (5)	158(4)
N2–H2N···Cl2[b]	0.88(3)	3.306(3)	2.44(3)	164 (2)
N1–H1N···Cl2[b]	0.90(3)	3.362(3)	2.51(3)	159 (2)
O5–H2W···Cl2[b]	0.82(3)	3.227(5)	2.48(5)	152 (3)

a) *x*, *y*–1, *z*; b) –*x*, *y*–1/2, –*z*+1/2;

Table SI 4. Hydrogen bonding geometry in **IV**.

D–H···A[operator]	*d*(D–H)	*d*(D···A)	*d*(H···A)	*φ*(D–H···A)
N1–H1N···O5	0.909(17)	2.980(3)	2.090(19)	166.1(1.5)
N2–H2N···O5	0.91(2)	3.199(4)	2.362(18)	153.0(1.5)
C10–H10···O3[a]	0.930	3.352(4)	2.677	130.12
C9–H9···O3[a]	0.930	3.493(4)	2.966	117.44
C12–H12B···O3[a]	0.970	3.399(2)	2.947	109.65
C11–H11A···O3[a]	0.970	3.485(3)	2.772	130.93
O5–H2W···Cl2[b]	0.72(4)	3.180(3)	2.46(4)	175(4)
C8–H8···O4[c]	0.930	3.418(2)	2.545	156.53
O5–H1W···Cl2[d]	0.79 (4)	3.105(3)	2.35(3)	166(3)

a) –*x*+1, –*y*+2, –*z*+2; b) –*x*+1, –*y*+2, –*z*+1; c) *x*–1, *y*, *z*+1; d) *x*+1, *y*, *z*

* In all the tables, the standars uncertanties for distances and angles involning hydrogen atoms placed on calculated positions have been omitted.

Table SI 5. Hydrogen bonding geometry in **V**.

D–H···A[operator]	*d*(D–H)	*d*(D···A)	*d*(H···A)	*φ*(D–H···A)
N1–H1N···Cl2	0.921	3.343(19)	2.443	165.62
O7–H2W···Cl2	0.839	3.571(15)	2.737	172.65
O7–H1W···Cl1[a]	0.840	3.211(11)	2.423	156.60
O7–H1W···Cl1[b]	0.840	3.211(11)	2.423	156.60

a) –*x*+1, –*y*, –*z*+1; b) –*x*+1, –*y*, *z*+1

Table SI 6. Hydrogen bonding geometry in **VI**.

D–H···A[operator]	*d*(D–H)	*d*(D···A)	*d*(H···A)	*φ*(D–H···A)
N2–H2A···Cl2	0.900	2.598(18)	1.729	161.49
O2–H2W···Cl1	0.894(17)	3.20 (3)	2.32(4)	171(3)
C14–H14B···O3[a]	0.969	3.162(5)	2.613	116.09
C13–H13B···O3[a]	0.971	3.404(5)	2.836	118.20
N1–H1N···Cl1[c]	0.91(2)	3.28(3)	2.37(3)	176.1(6)
O2–H1W···Cl2[d]	0.89(6)	3.09(3)	2.21(5)	166(4)

a) *x*+1/2, *y*+1/2, *z*–1; b) *x*, *y*, *z*+1; c) *x*, –*y*+1, *z*+1; d) *x*–1, *y*, *z*+1

Table SI 7. Hydrogen bonding geometry in **VII**.

D–H···A[operator]	*d*(D–H)	*d*(D···A)	*d*(H···A)	*φ*(D–H···A)
N1–H1N···O7[a]	0.909(16)	3.275(3)	2.399(16)	161.8(1.2)
N1–H1N···O6[a]	0.909(16)	3.104(4)	2.32(2)	144.4(1.4)
N2–H2N···O7[a]	0.909(18)	3.578(3)	2.839(19)	139.4(1.3)
N2–H2N···O6[a]	0.909(18)	2.981(3)	2.078(19)	172.7(1.6)
C7–H7···O4[b]	0.930	3.277(4)	2.592	130.86
C8–H8···O4[b]	0.929	3.405(4)	2.858	118.83

a) –*x*+3/2, *y*–1/2, –*z*+3/2; b) –*x*+3/2, *y*+1/2, –*z*+3/2

Table SI 8. Hydrogen bonding geometry in **VIII**.

D–H···A[operator]	*d*(D–H)	*d*(D···A)	*d*(H···A)	*φ*(D–H···A)
C3–H3···O2[a]	0.930	3.299(4)	2.532	140.05
N1–H1N···S2[b]	0.908(18)	3.476(2)	2.579(19)	169.5(1.3)

a) –*x*, –*y*, –*z*+1; b) *x*–1, *y*, *z*

Table SI 9. Hydrogen bonding geometry in **IX**.

D–H···A[operator]	*d*(D–H)	*d*(D···A)	*d*(H···A)	*φ*(D–H···A)
N2–H2···S1[a]	0.911	3.557(7)	2.712	154.85
N1–H1···S1[a]	0.911	3.527(7)	2.681	155.05

a) *x*, *y*, *z*–1

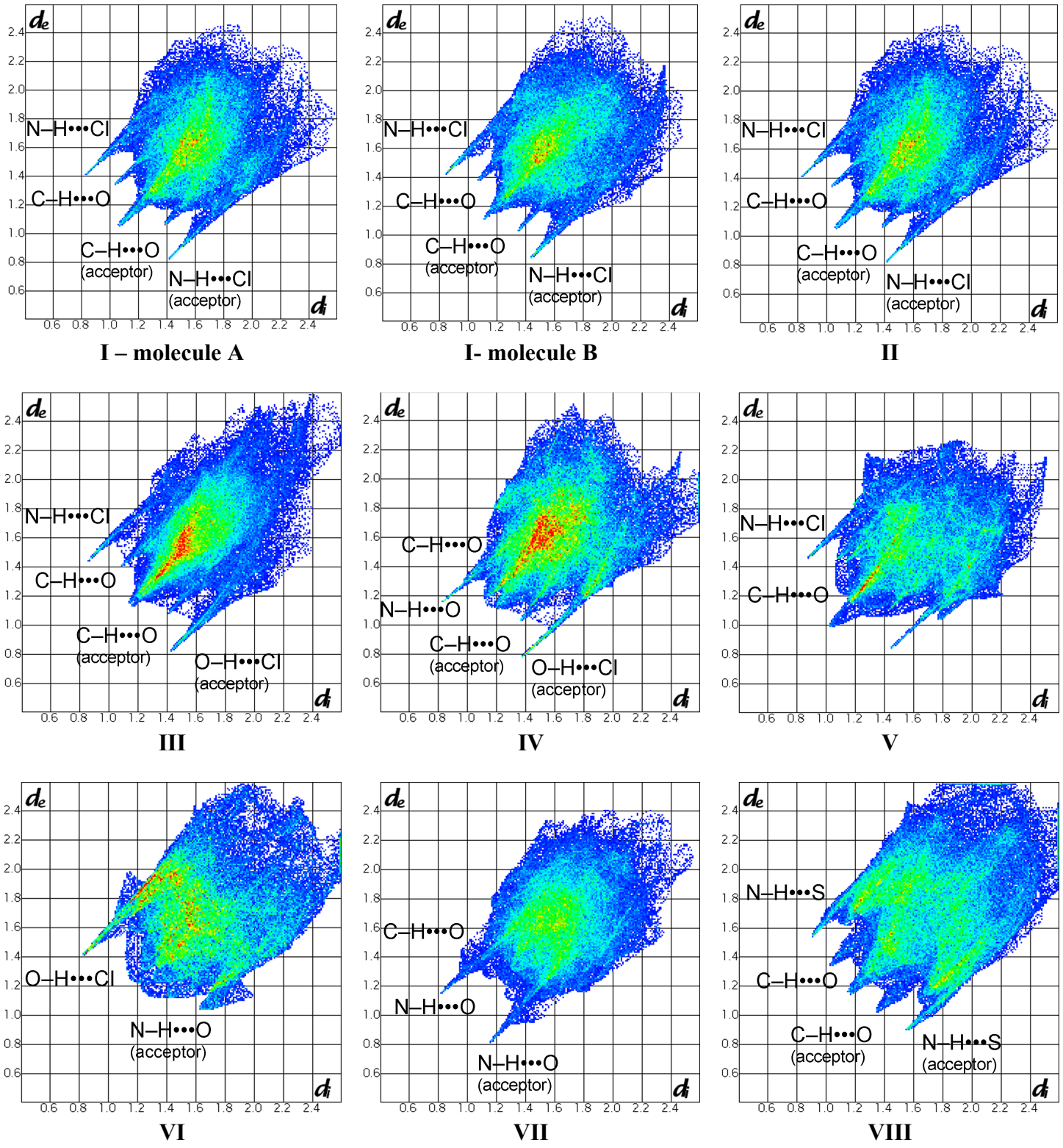
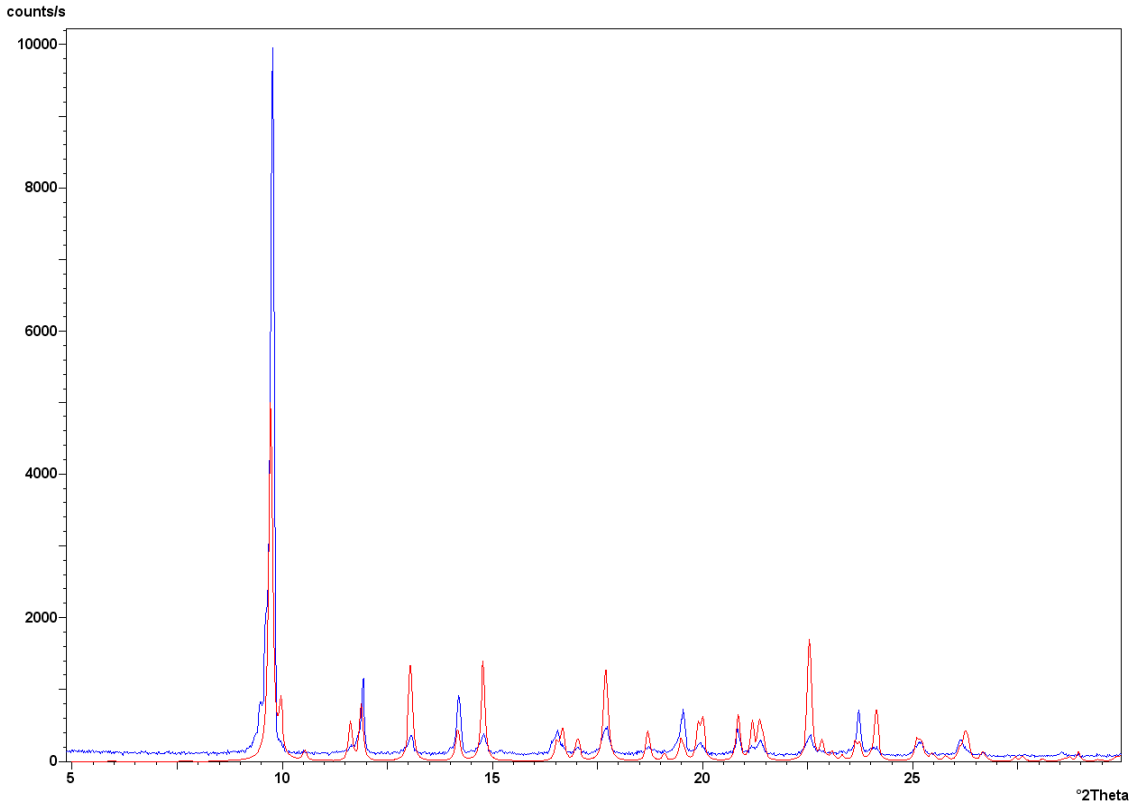
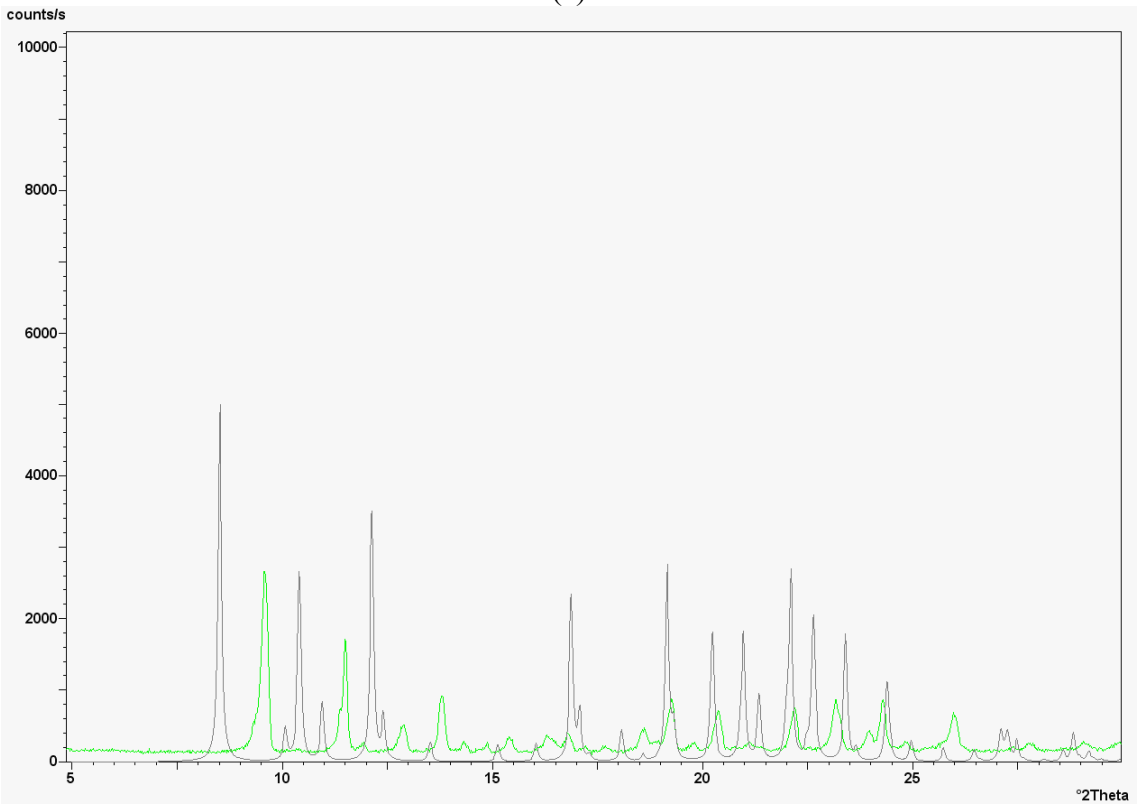


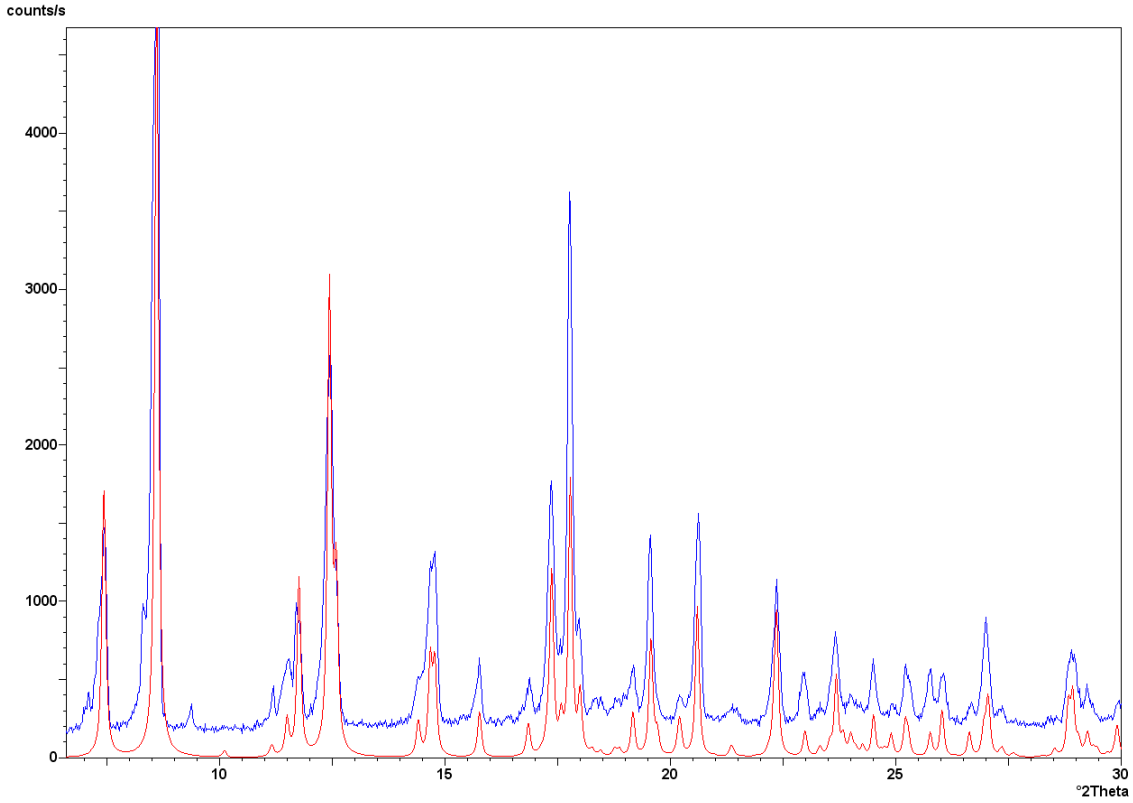
Figure S10. Hirshfeld-surfaces fingerprint plots for copper(II) coordination moieties.



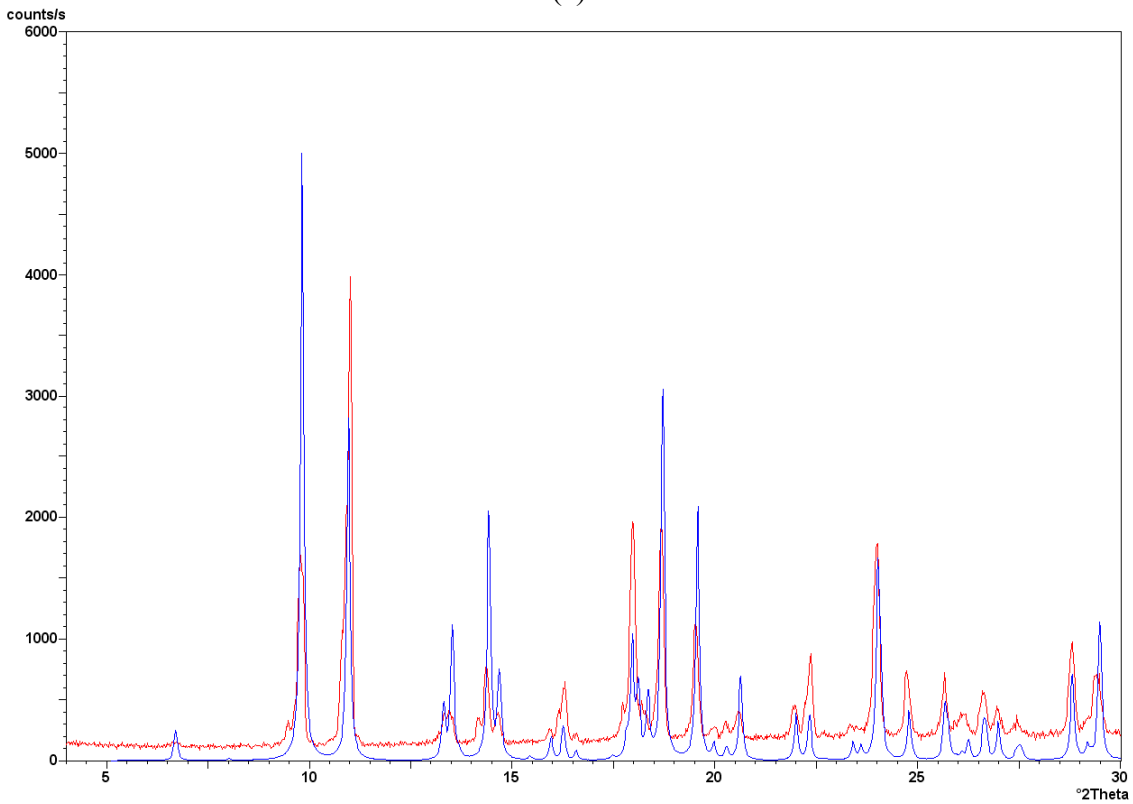
(a)



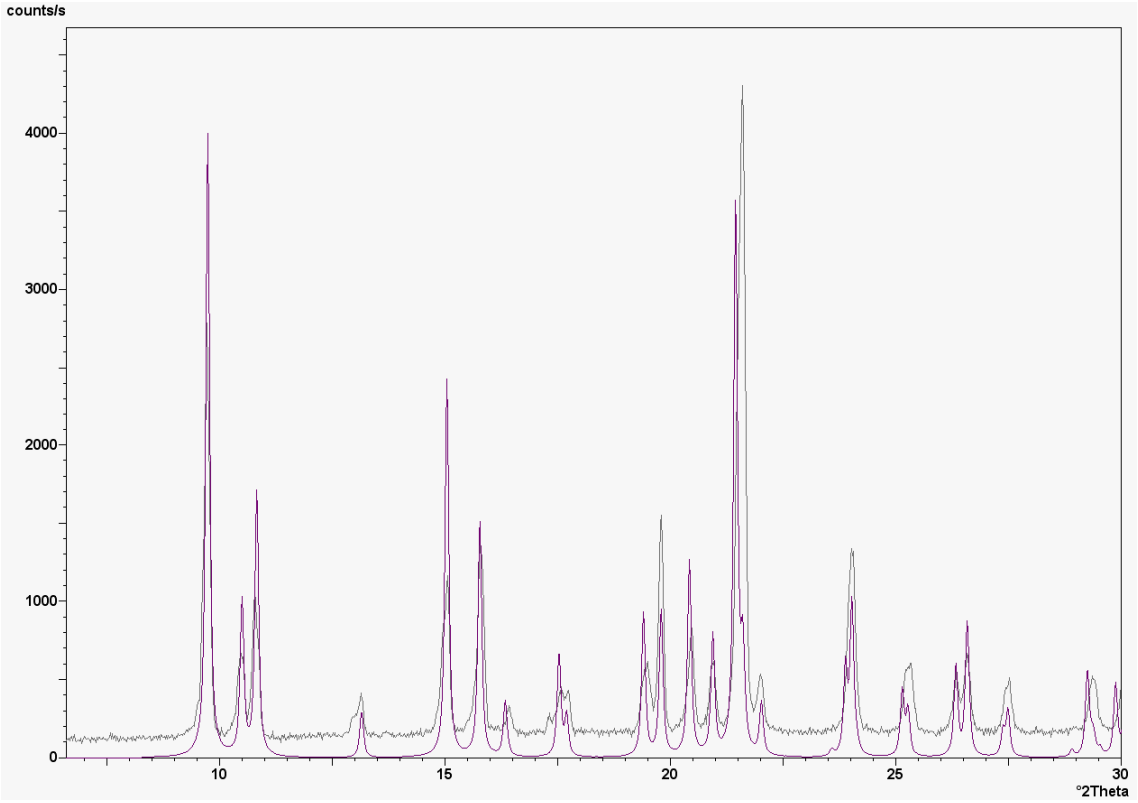
(b)



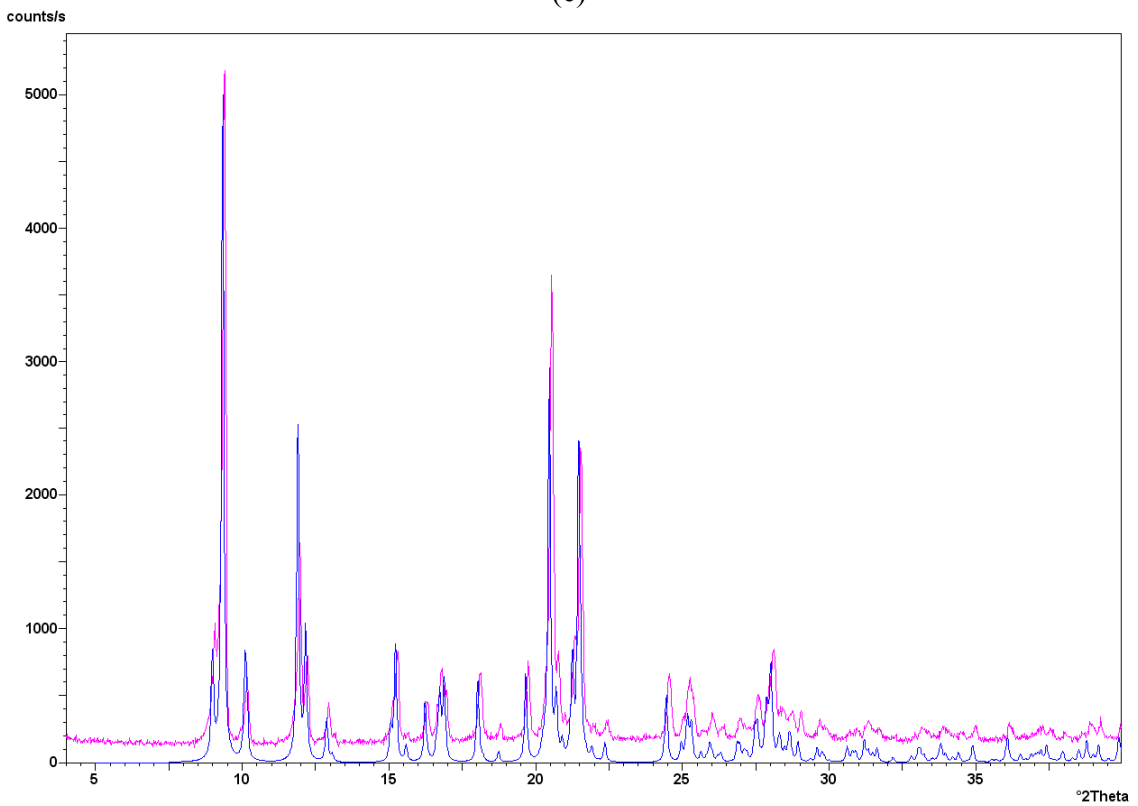
(c)



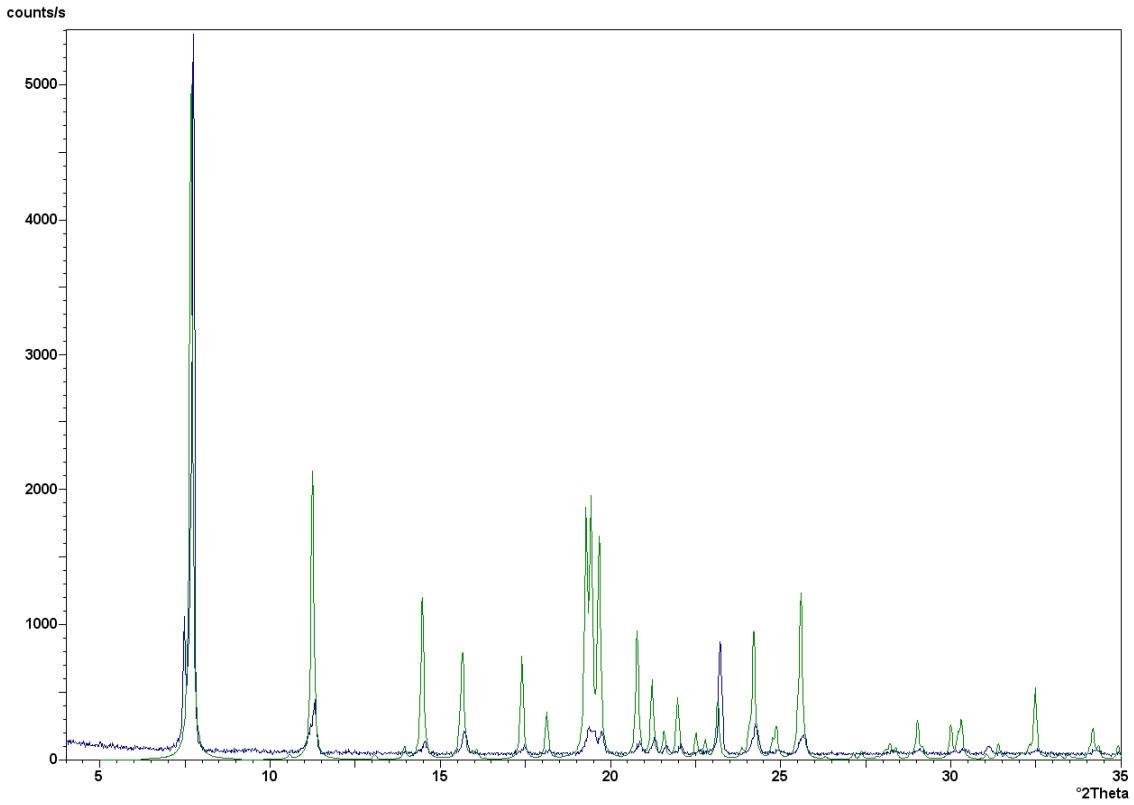
(d)



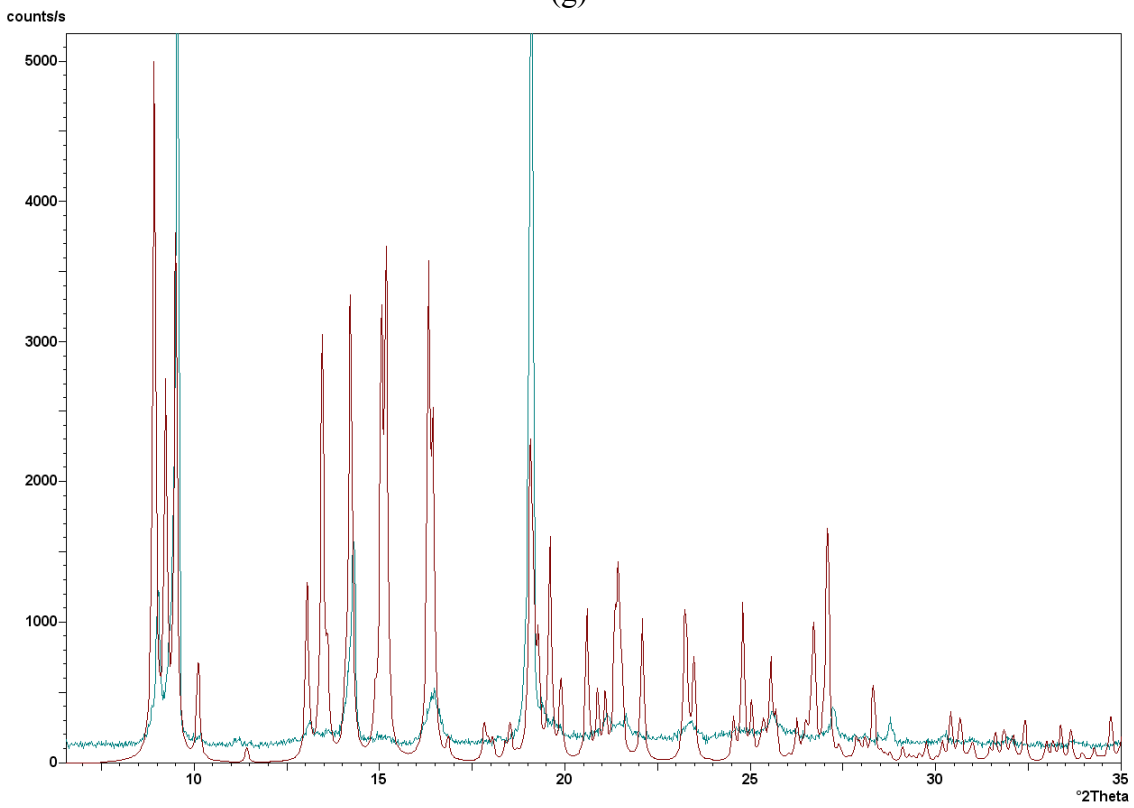
(e)



(f)

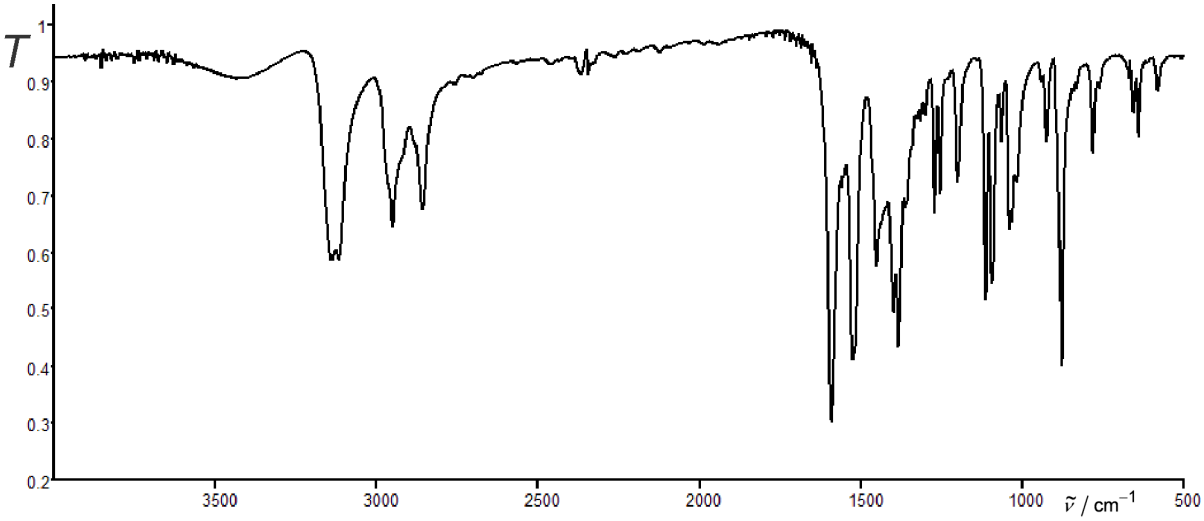


(g)

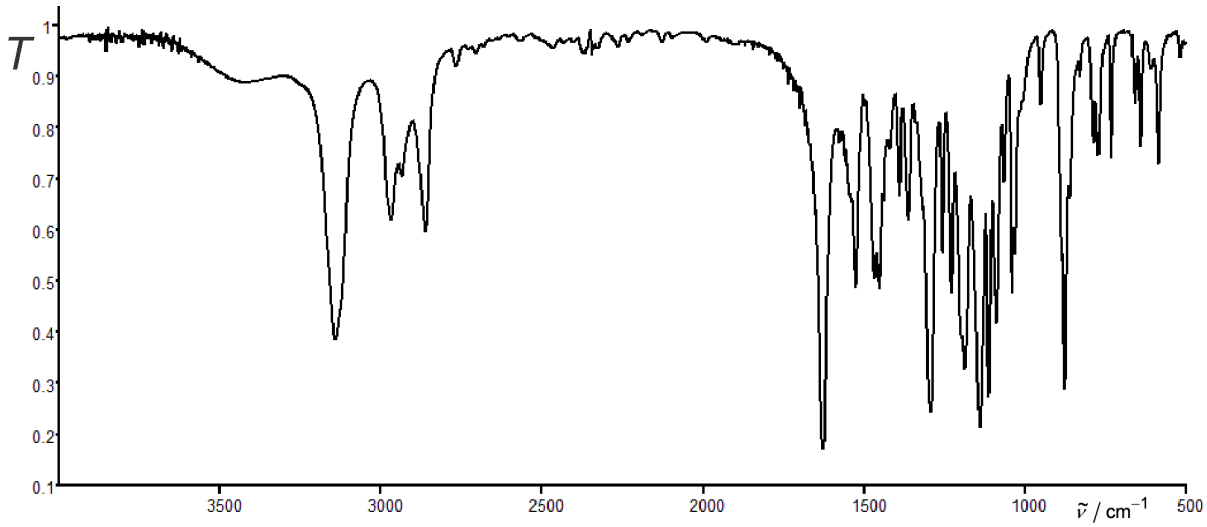


(h)

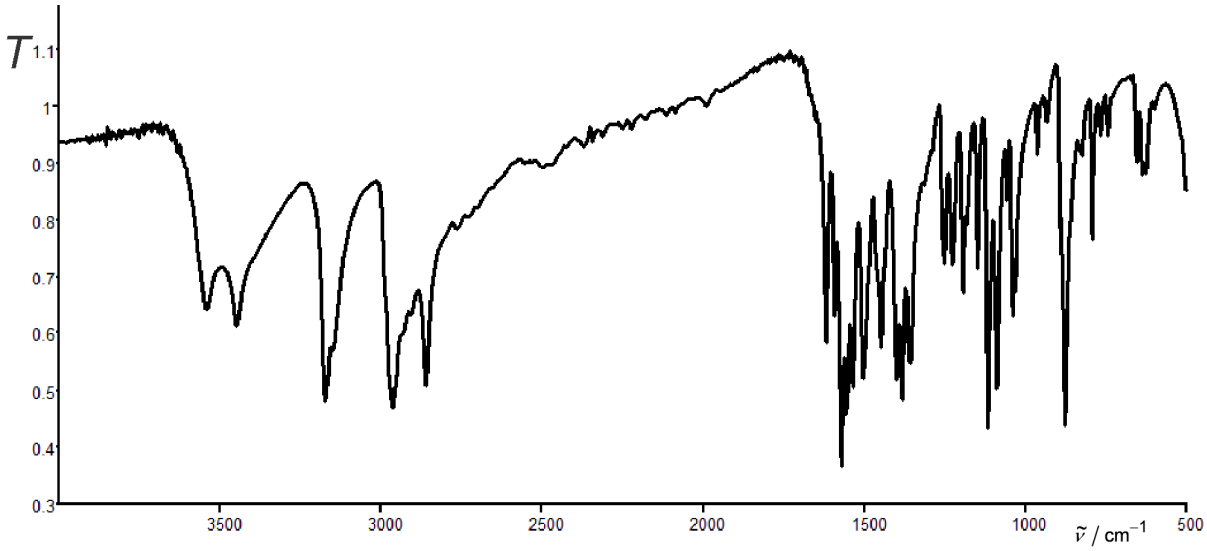
Figure S11. Comparison of experimental and calculated PXRD patterns for a) **I** (blue – experimental, red-calculated); b) **II** ((green – experimental, grey-calculated); c) **III** (blue – experimental, red-calculated); d) **IV** (red – experimental, blue-calculated); e) **V** (grey – experimental, purple-calculated); f) **VII** (red – experimental, blue-calculated); g) **VIII** (blue – experimental, green-calculated); h) **IX** (blue – experimental, red-calculated). VI was not included due to the immediate solvent egress at room temperature and consequent decomposition of the sample.



(a)

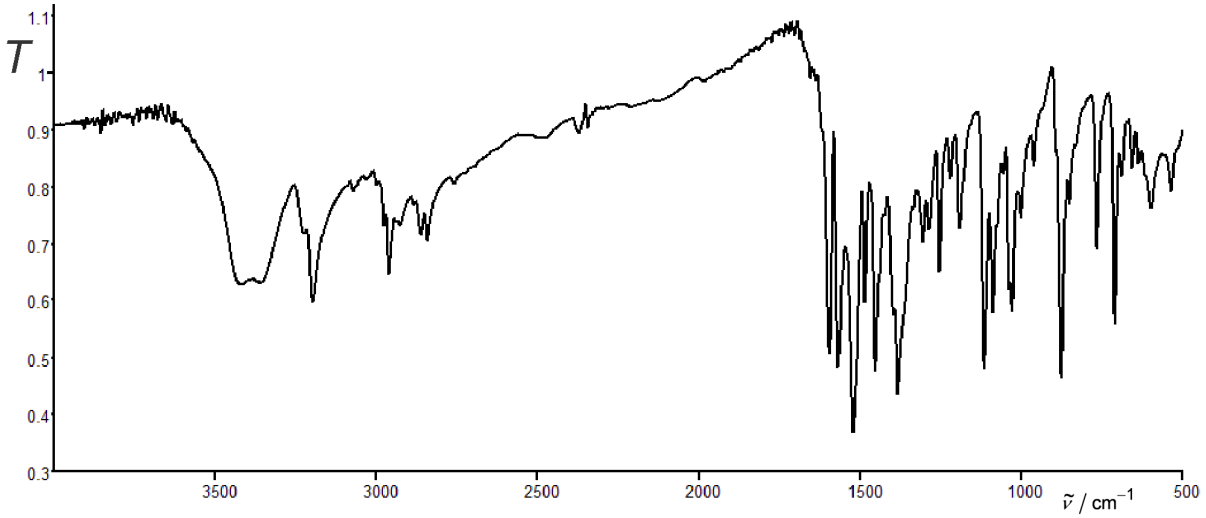


(b)

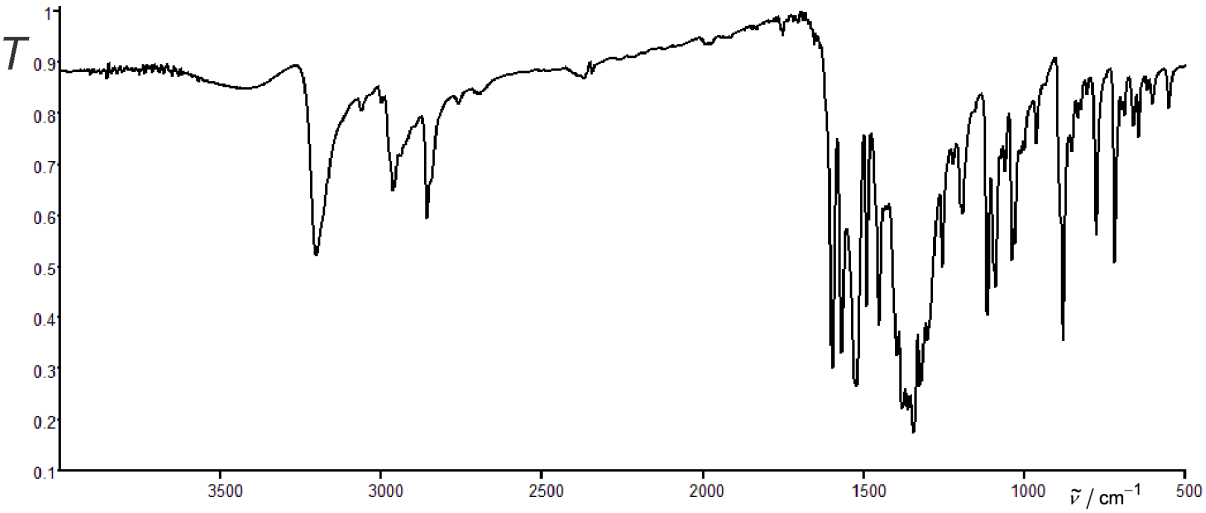


(c)

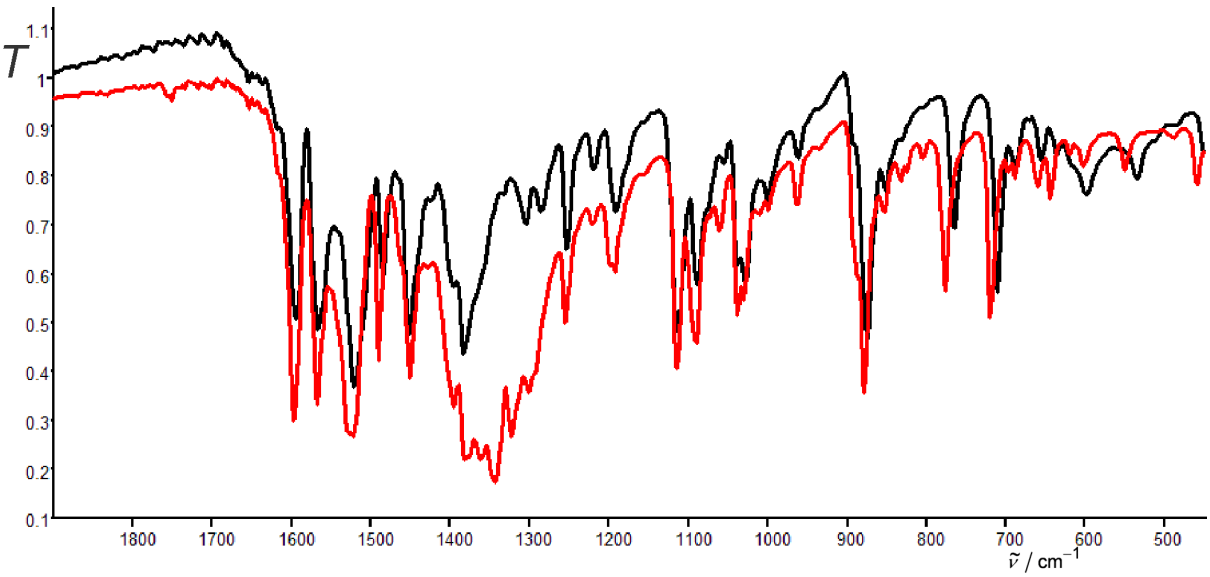
Figure S12. Infrared spectra (KCl pellet, 4000–500 cm^{-1}) for compounds **I** (a), **II** (b), and **III** (c).



(a)

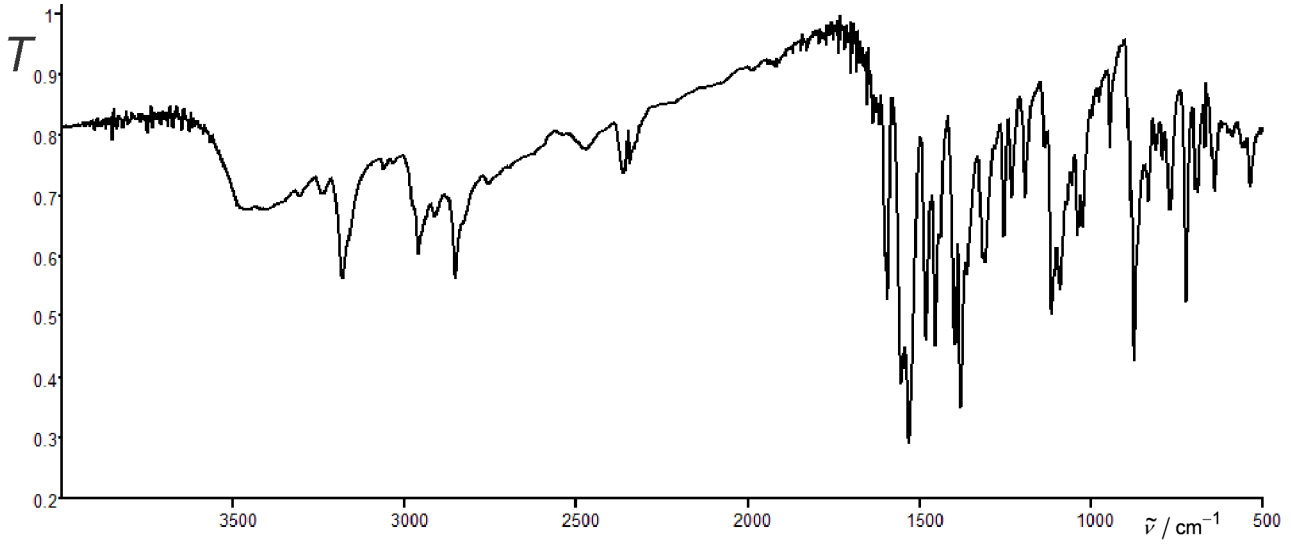


(b)

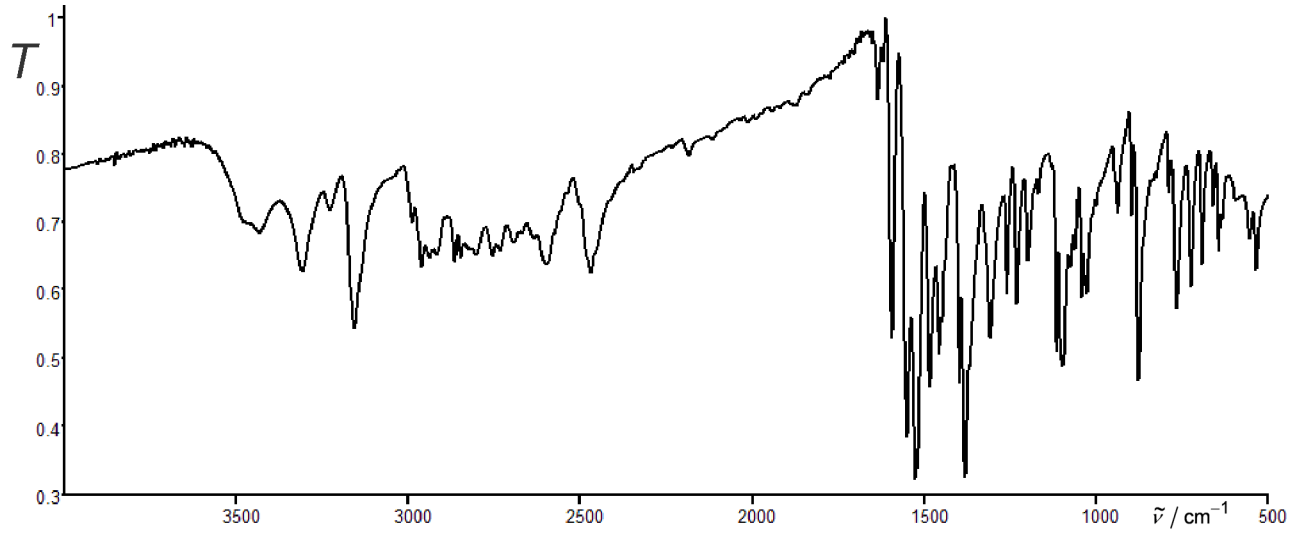


(c)

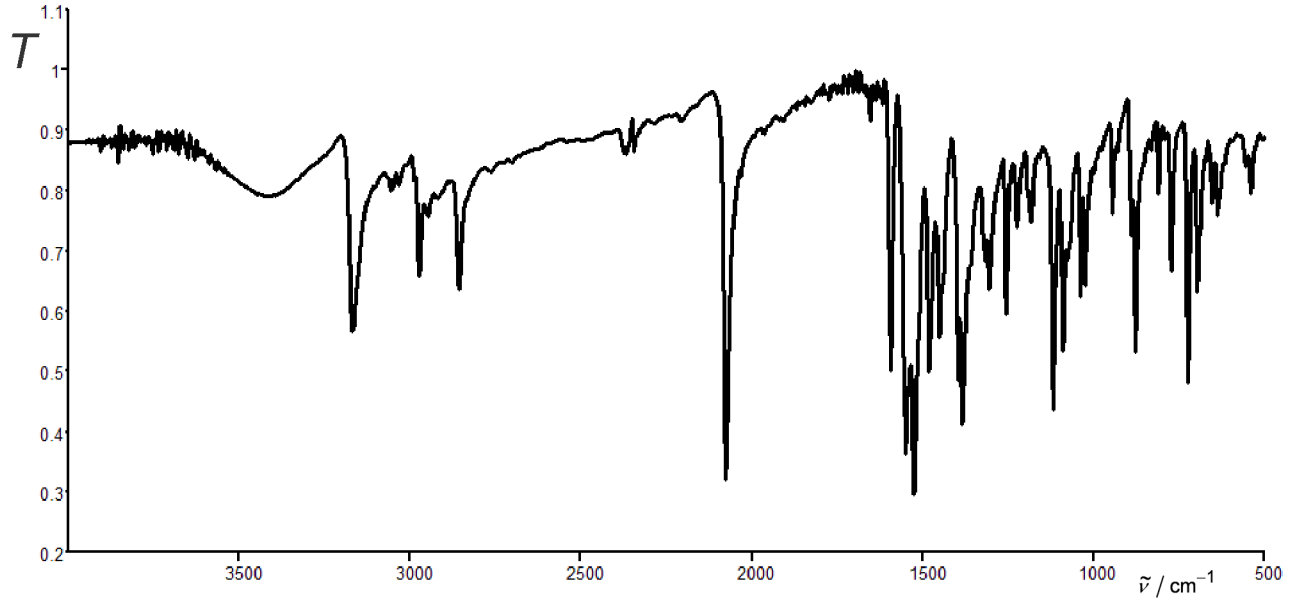
Figure S12. Infrared spectra (KCl pellet, 4000–500 cm^{-1}) for compounds **IV** (a) and **VII** (b); c) Infrared-spectra overlap (KCl pellet, 2000–500 cm^{-1}) for compounds **IV** (black) and **VII** (red).



(a)

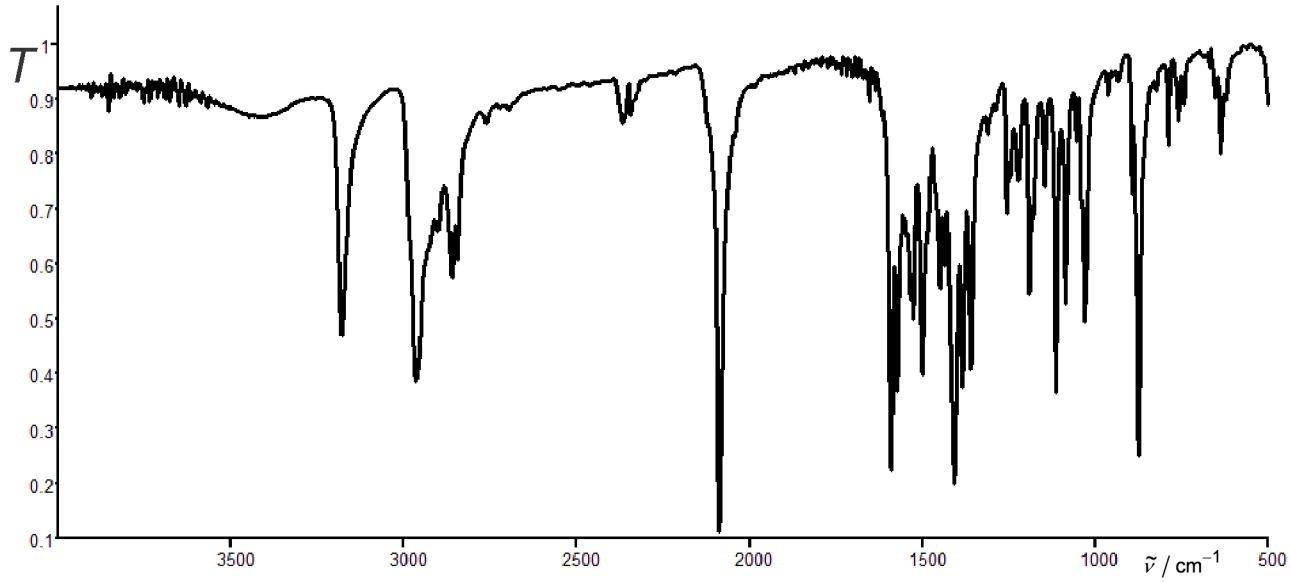


(b)

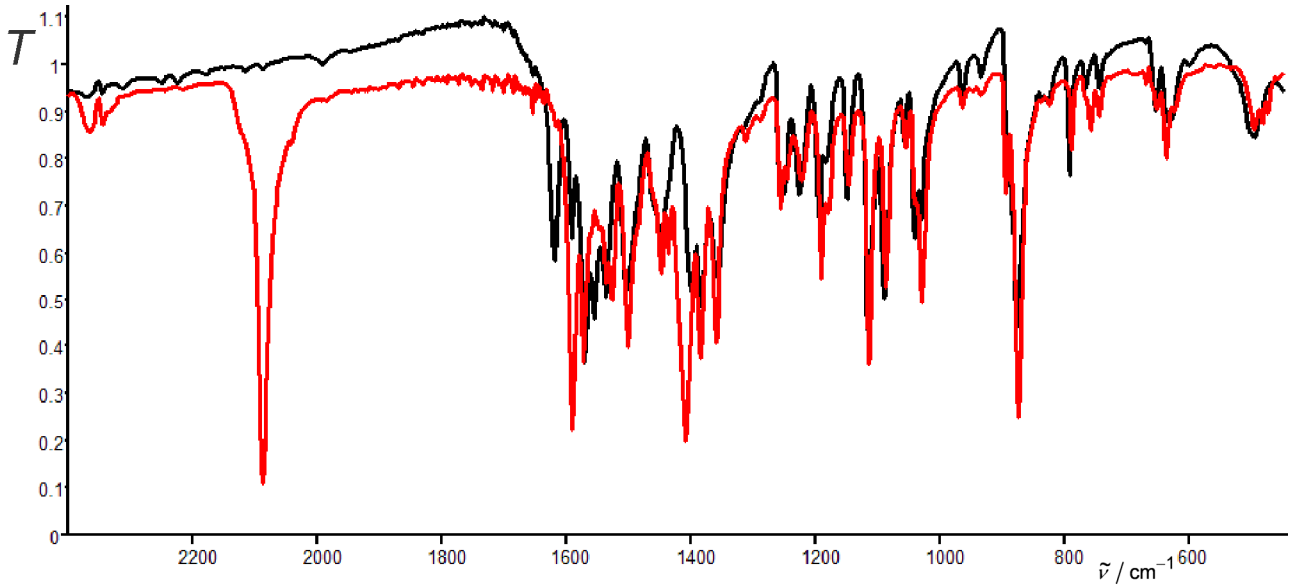


(c)

Figure S12. Infrared spectra (KCl pellet, 4000–500 cm^{-1}) for compounds **V** (a), **VI** (b), and **VIII** (c).



(a)



(b)

Figure S12. a) Infrared spectra (KCl pellet, 4000–500 cm^{-1}) for compound **IX**; b) Infrared-spectra overlap (KCl pellet, 2400–500 cm^{-1}) for compounds **III** (black) and **IX** (red).