Supporting information for

Structural diversity and magnetic properties of copper(II) quinaldinate compounds with amino alcohols

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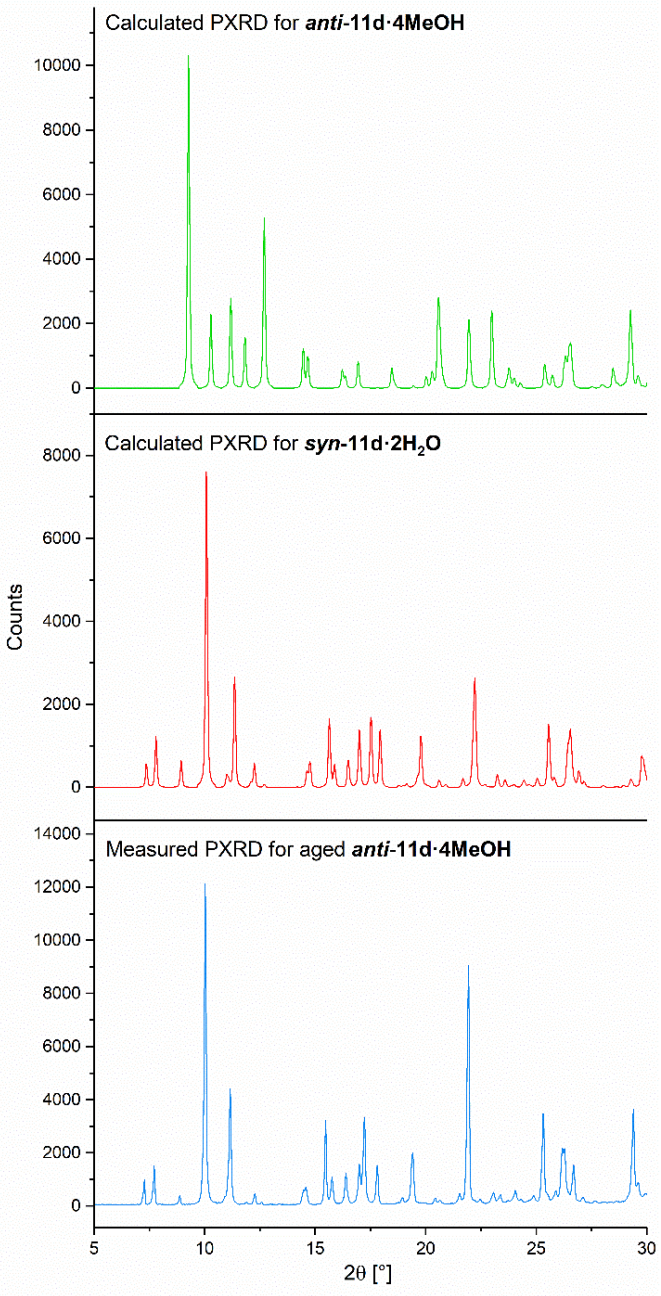
1. Powder X-ray diffraction

Figure S1. Comparison of the calculated powder patterns for ***anti*-11d·4MeOH** (green line, 150 K) and ***syn*-11d·2H₂O** (red, 150 K) with the measured PXRD pattern for the aged ***anti*-11d·4MeOH** (blue, room temperature).



2. Single-crystal X-ray structure determinations

Table S1. Crystallographic data for **1a** to **8b**.

	1a	**2b**	**g**	***anti*-4d**	**5e**	**6a**	**7a**	**7e**	**8b**
Empirical formula	$C_{24}H_{26}CuN_4O_6$	$C_{23}H_{21}CuN_3O_5$	$C_{20}H_{12}CuN_2O_4$	$C_{28}H_{32}Cu_2N_4O_6$	$C_{29}H_{39}CuN_5O_7$	$C_{28}H_{34}CuN_4O_6$	$C_{28}H_{34}CuN_4O_6$	$C_{32}H_{45}CuN_5O_7$	$C_{23}H_{21}CuN_3O_5$
Formula weight	530.03	482.97	407.86	647.65	633.19	586.13	586.13	675.27	482.97
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	triclinic	triclinic	triclinic	triclinic
Space group	$P\,2_1/n$	$C\,2/c$	$P\,2_1/c$	$P\,2_1/c$	$P\,\bar{1}$	$P\,\bar{1}$	$P\,\bar{1}$	$P\,\bar{1}$	$P\,\bar{1}$
***T* [K]**	150.00(10)	150.00(10)	150.00(10)	150.00(10)	150.00(10)	150.00(10)	150.00(10)	150.00(10)	150.00(10)
λ [Å]	1.54184	1.54184	0.71073	0.71073	1.54184	1.54184	1.54184	0.71073	0.71073
***a* [Å]**	9.8103(3)	19.2147(5)	4.8617(2)	7.3120(4)	9.3197(4)	6.0630(3)	5.8410(3)	11.3901(5)	8.8642(6)
***b* [Å]**	5.9728(2)	7.9105(2)	13.5497(5)	20.7381(11)	12.5306(7)	10.1393(4)	9.7548(4)	12.8020(6)	10.1622(6)
***c* [Å]**	19.2540(5)	14.0321(4)	12.2556(4)	8.8408(4)	14.6852(7)	10.9316(4)	11.6529(5)	13.0487(6)	13.7176(8)
α [°]	90	90	90	90	106.796(5)	87.176(3)	92.222(4)	66.301(4)	106.140(5)
β [°]	98.697(3)	107.901(3)	96.467(3)	98.162(5)	94.775(4)	84.072(3)	91.154(4)	70.763(4)	93.452(5)
γ [°]	90	90	90	90	110.018(4)	88.091(3)	91.002(4)	87.575(4)	115.573(6)
***V* [Å^3]**	1115.22(6)	2029.60(10)	802.20(5)	1327.01(12)	1510.64(14)	667.34(5)	663.21(5)	1636.01(14)	1047.28(12)
Z	2	4	2	2	2	1	1	2	2
D_{calc} [g/cm^3]	1.578	1.581	1.689	1.621	1.392	1.458	1.468	1.371	1.532
μ [mm^{-1}]	1.822	1.890	1.393	1.654	1.469	1.577	1.587	0.721	1.085
Collected reflections	5193	11965	12501	6747	11079	11908	11209	16213	10446
Unique reflections	2266	2071	2202	3448	6067	2730	2699	8449	5431
Observed reflections	1991	1874	1987	2621	4803	2520	2412	6150	4708
R_{int}	0.0282	0.0290	0.0283	0.0354	0.0376	0.0526	0.0527	0.0341	0.0254
R_1 ($I > 2\sigma(I)$)	0.0308	0.0307	0.0263	0.0445	0.0452	0.0358	0.0372	0.0490	0.0367
wR_2 (all data)	0.0862	0.0852	0.0711	0.1241	0.1234	0.0934	0.1016	0.1109	0.0840

Table S2. Crystallographic data for **8c** to **11b**.

	8c	***syn*-8d**	**8e**	**9f**	**10e**	**11a**	**11a·3a1pOH**	**11b**
Empirical formula	$C_{23}H_{21}CuN_3O_5$	$C_{26}H_{28}Cu_2N_4O_6$	$C_{29}H_{39}CuN_5O_7$	$C_{36}H_{56}CuN_6O_8$	$C_{32}H_{45}CuN_5O_7$	$C_{26}H_{30}CuN_4O_6$	$C_{29}H_{39}CuN_5O_7$	$C_{23}H_{21}CuN_3O_5$
Formula weight	482.97	619.60	633.19	764.40	675.27	558.08	633.19	482.97
Crystal system	monoclinic	monoclinic	triclinic	triclinic	triclinic	triclinic	triclinic	monoclinic
Space group	$P\,2_1/n$	$I\,2/a$	$P\,1$	$P\,\bar{1}$	$P\,\bar{1}$	$P\,\bar{1}$	$P\,\bar{1}$	$I\,2/a$
***T* [K]**	150.00(10)	150.00(10)	150.00(10)	150.00(10)	150.00(10)	150.00(10)	150.00(10)	150.00(10)
λ [Å]	0.71073	0.71073	0.71073	0.71073	0.71073	1.54184	0.71073	1.54184
***a* [Å]**	10.2710(6)	9.6201(6)	11.0057(3)	8.1133(4)	14.1491(5)	5.6066(3)	7.4853(3)	13.8822(4)
***b* [Å]**	7.6001(4)	23.1763(18)	11.4891(4)	10.3368(5)	21.7604(9)	10.4353(6)	14.1745(6)	8.3669(2)
***c* [Å]**	13.5989(8)	11.8397(11)	12.6324(4)	12.0359(5)	23.6679(9)	11.2830(7)	14.3105(6)	18.7238(5)
α [°]	90	90	81.107(3)	81.030(4)	110.376(4)	104.885(5)	88.622(3)	90
β [°]	108.617(6)	99.147(7)	79.836(3)	83.371(4)	100.665(3)	95.480(5)	76.298(4)	111.589(3)
γ [°]	90	90	73.162(3)	72.014(4)	91.832(3)	99.643(4)	82.897(3)	90
***V* [Å^3]**	1005.99(10)	2606.2(4)	1495.73(9)	945.89(8)	6676.3(5)	622.28(6)	1463.80(11)	2022.22(10)
Z	2	4	2	1	8	1	2	4
D_{calc} [g/cm^3]	1.594	1.579	1.406	1.342	1.344	1.489	1.437	1.586
μ [mm^{-1}]	1.129	1.681	0.784	0.635	0.707	1.662	0.801	1.897
Collected reflections	5118	7957	26975	16937	68809	4819	13494	3761
Unique reflections	2606	3010	15312	5069	34714	2524	7569	2028
Observed reflections	2091	2011	13229	4523	16450	2437	6185	1975
R_{int}	0.0282	0.0701	0.0253	0.0292	0.0583	0.0235	0.0209	0.0148
R_1 ($I > 2\sigma(I)$)	0.0359	0.0571	0.0440	0.0336	0.0684	0.0340	0.0379	0.0322
wR_2 (all data)	0.0910	0.1214	0.1079	0.0877	0.1749	0.0933	0.1047	0.0904

Table S3. Crystallographic data for **11c** to ***anti*-11d·2MeOH·2(3a1pOH)**.

	11c	***syn*-11d**	***syn*-11d·2H$_2$O**	***anti*-11d·2MeCN**	***anti*-11d·4MeOH**	***anti*-11d·2MeOH·2(3a1pOH)**
Empirical formula	$C_{23}H_{21}CuN_3O_5$	$C_{26}H_{28}Cu_2N_4O_6$	$C_{26}H_{32}Cu_2N_4O_8$	$C_{30}H_{34}Cu_2N_6O_6$	$C_{30}H_{44}Cu_2N_4O_{10}$	$C_{34}H_{54}Cu_2N_6O_{10}$
Formula weight	482.97	619.60	655.63	701.71	747.77	833.91
Crystal system	monoclinic	triclinic	triclinic	monoclinic	monoclinic	monoclinic
Space group	$P\,2_1/n$	$P\,\bar{1}$	$P\,\bar{1}$	$P\,2_1/n$	$P\,2_1/n$	$P\,2_1/c$
***T* [K]**	150.00(10)	150.00(10)	150.00(10)	150.00(10)	150.00(10)	150.00(10)
λ [Å]	1.54184	0.71073	0.71073	1.54184	0.71073	0.71073
***a* [Å]**	10.3764(5)	9.5521(5)	10.0507(4)	10.2380(3)	10.9996(4)	12.0521(4)
***b* [Å]**	7.5417(4)	10.1620(5)	11.5520(5)	12.0196(4)	12.0720(3)	12.0235(3)
***c* [Å]**	13.4913(6)	14.8273(10)	12.1515(6)	12.4708(4)	12.8700(4)	14.0783(6)
α [°]	90	72.689(5)	82.366(4)	90	90	90
β [°]	107.782(5)	75.638(5)	83.857(4)	101.731(3)	107.881(3)	110.038(4)
γ [°]	90	66.350(5)	81.000(4)	90	90	90
***V* [Å^3]**	1005.33(9)	1244.97(14)	1375.77(11)	1502.56(8)	1626.42(9)	1916.57(12)
Z	2	2	2	2	2	2
D_{calc} [g/cm^3]	1.595	1.653	1.583	1.551	1.527	1.445
μ [mm^{-1}]	1.908	1.759	1.602	2.199	1.369	1.172
Collected reflections	4037	11625	13264	6232	16107	23793
Unique reflections	2013	6377	6877	3028	4433	5314
Observed reflections	1830	5071	5679	2753	3901	4428
R_{int}	0.0199	0.0266	0.0267	0.0226	0.0247	0.0304
R_1 ($I > 2\sigma(I)$)	0.0345	0.0337	0.0368	0.0312	0.0264	0.0282
wR_2 (all data)	0.0974	0.0827	0.0909	0.0860	0.0674	0.0677

Figure S2. ORTEP drawing of *trans*-[Cu(quin)$_2$(2aeOH)$_2$] (**1a**). Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radii.

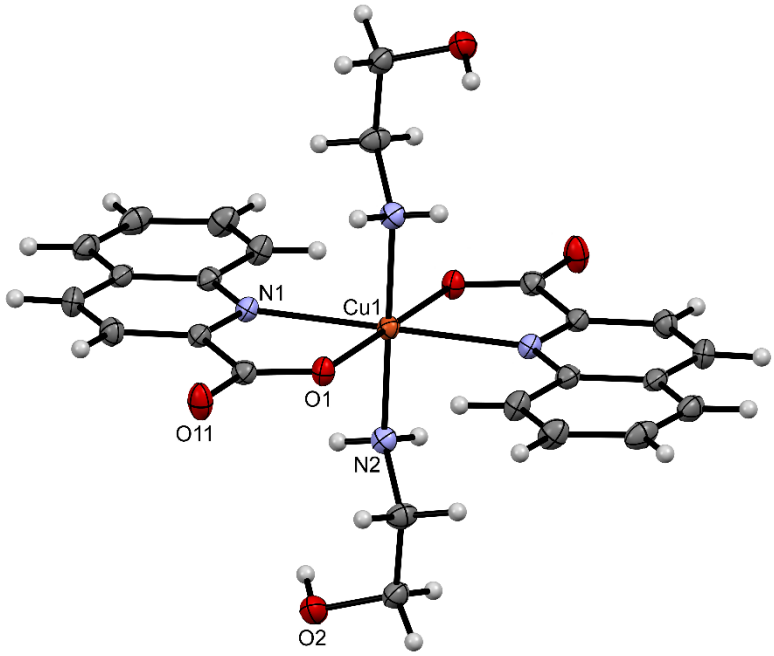


Figure S3. ORTEP drawing of *syn*-[Cu$_2$(quin)$_2$(2a1pO)$_2$] (***syn*-8d**). Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity.

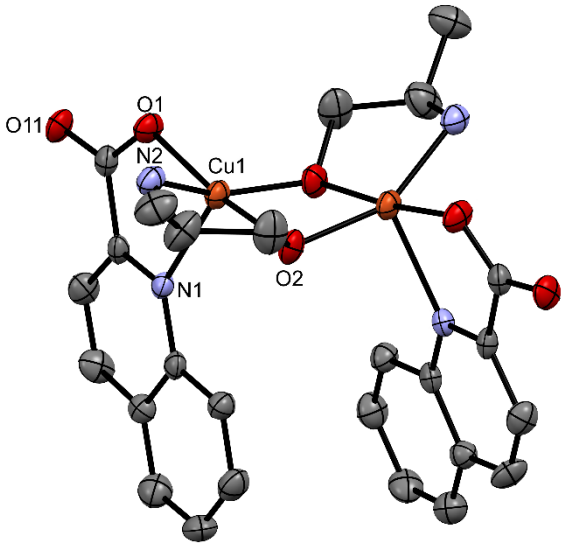


Figure S4. Views of the supramolecular chains in **1a** (top) and **11a** (bottom) showing the hydrogen bonding motifs.

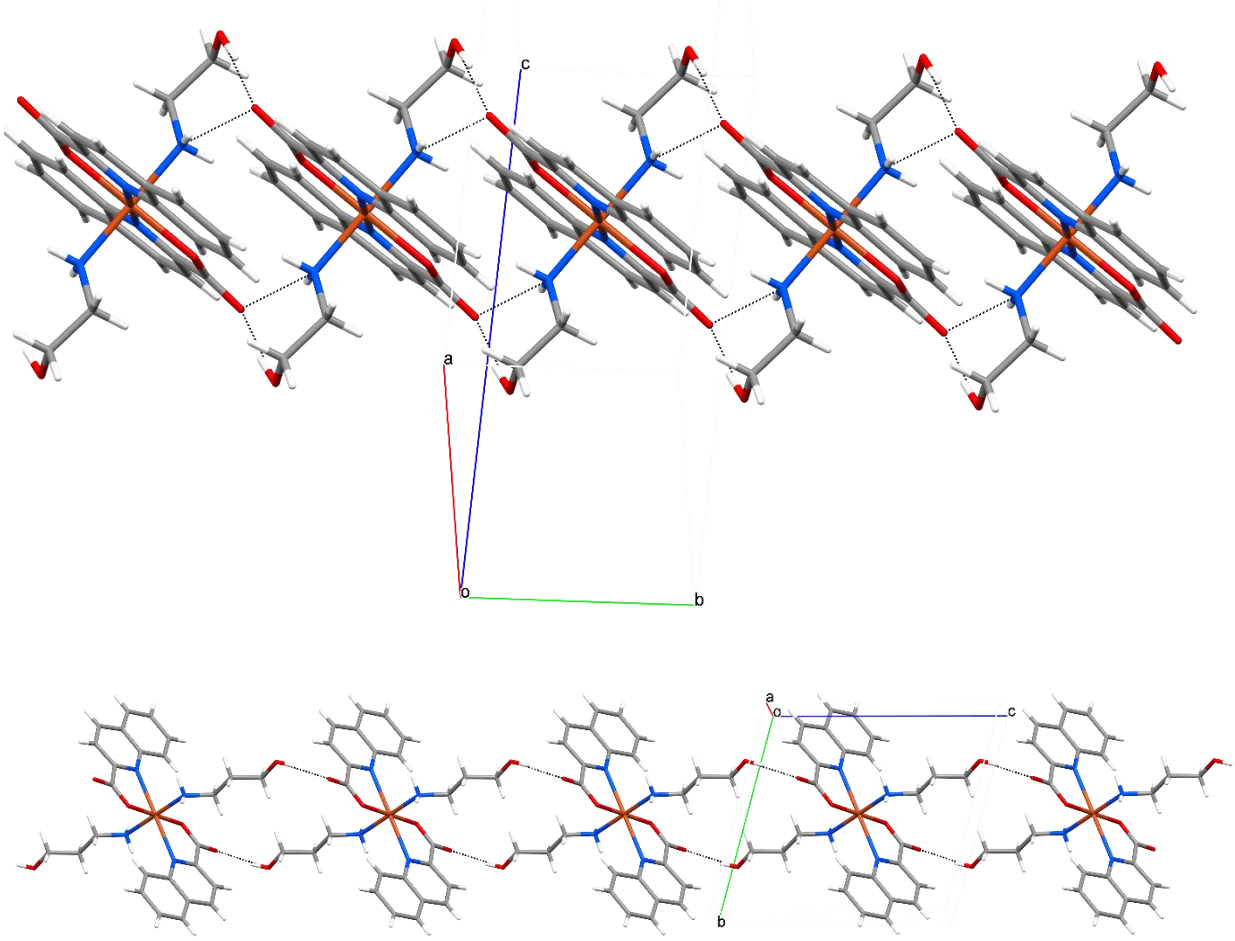


Figure S5. View of the supramolecular chain in **6a** (top) showing the $NH_2\cdots COO^-$ and $OH\cdots COO^-$ synthons, described in graph set notation as $C_1^1(6)$ and $C_1^1(9)$, respectively.[1]

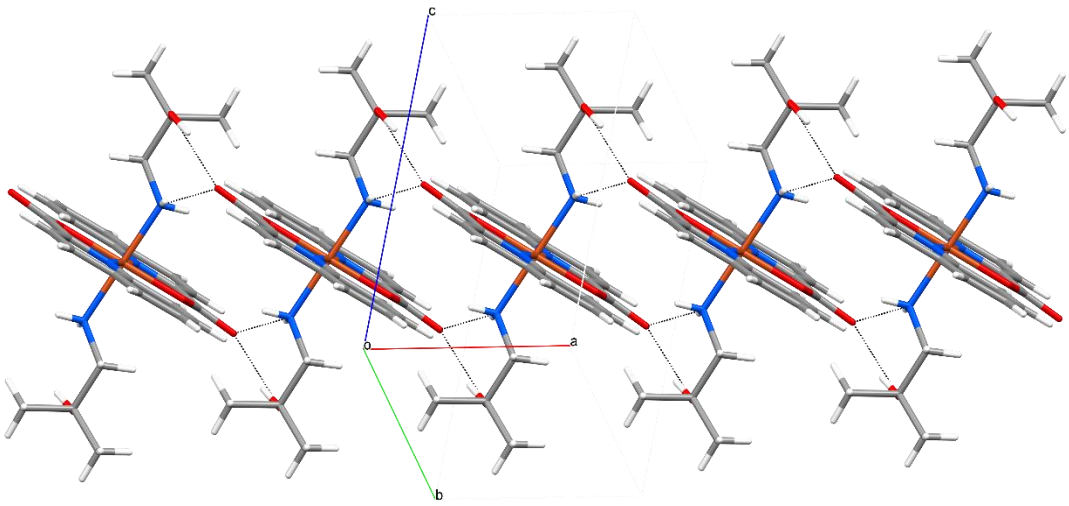
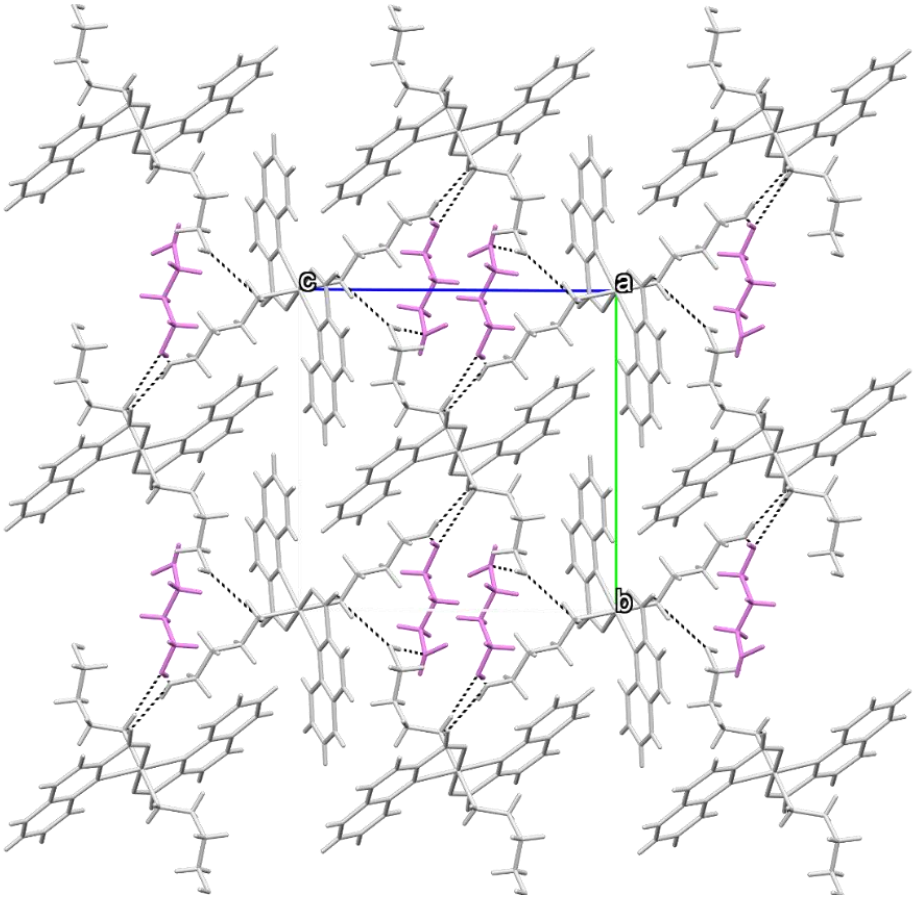


Figure S6. Hydrogen bonding in **11a·3a1pOH**: a projection along *a*-axis. Colour code: light grey - complex molecules, violet - 3a1pOH molecules.



[1] M. C. Etter, J. C. MacDonald and J. Bernstein, *Acta Crystallogr., Sect. B*, 1990, **46**, 256-262.

Figure S7. View of the supramolecular chain in **11b**.

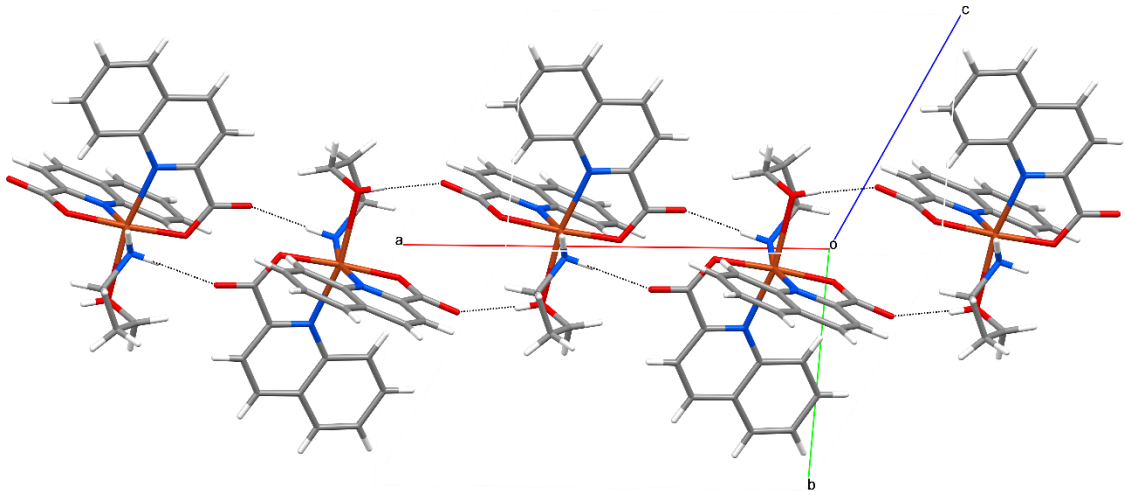


Figure S8. Views of the solid-state structure of **8c** showing a section of the chain running along *b*-axis (top) and the supramolecular layer (bottom). The bidentate bridging amino alcohol is disordered over two positions.

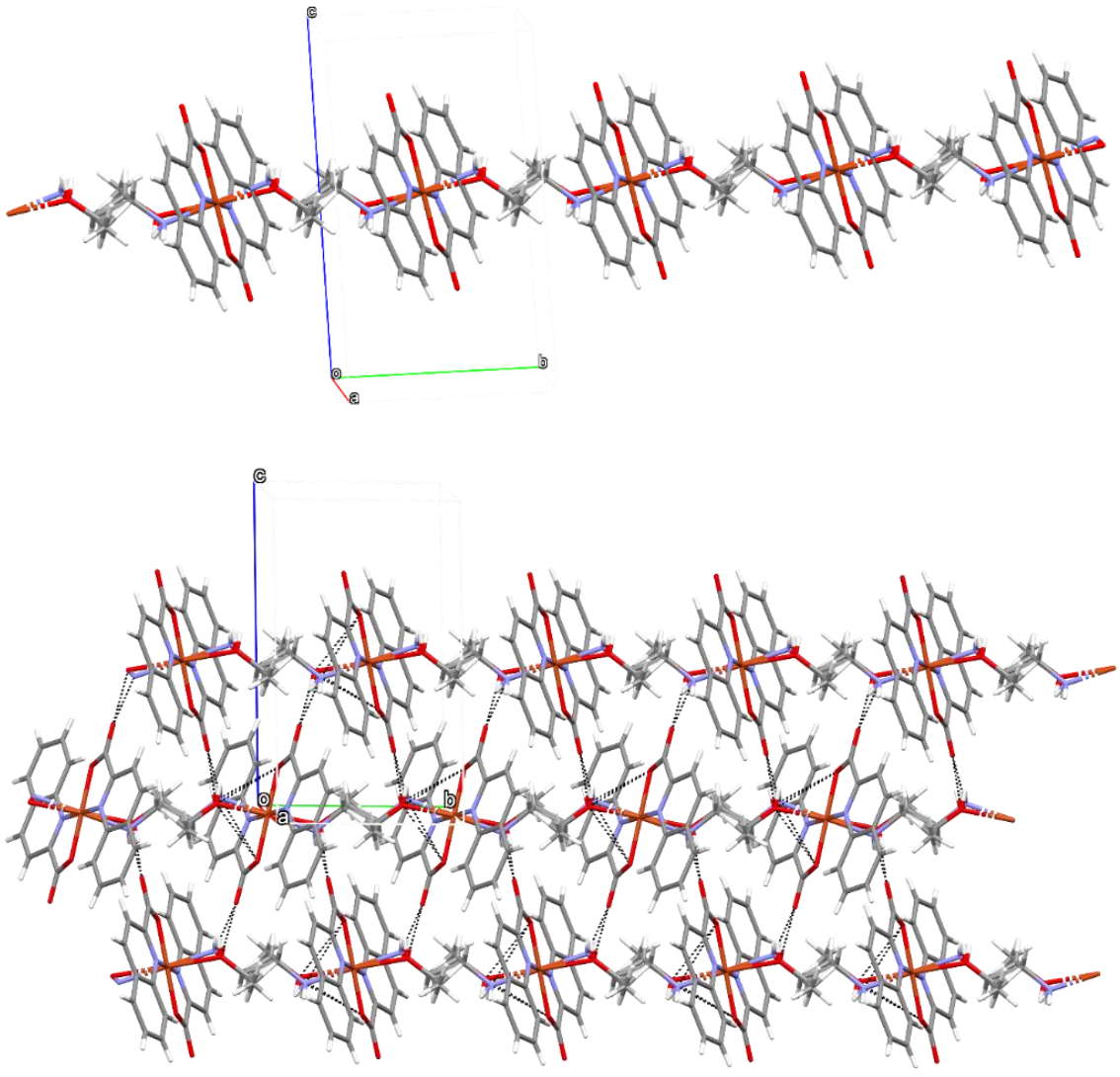


Figure S9. View of the supramolecular chain in ***syn*-8d**.

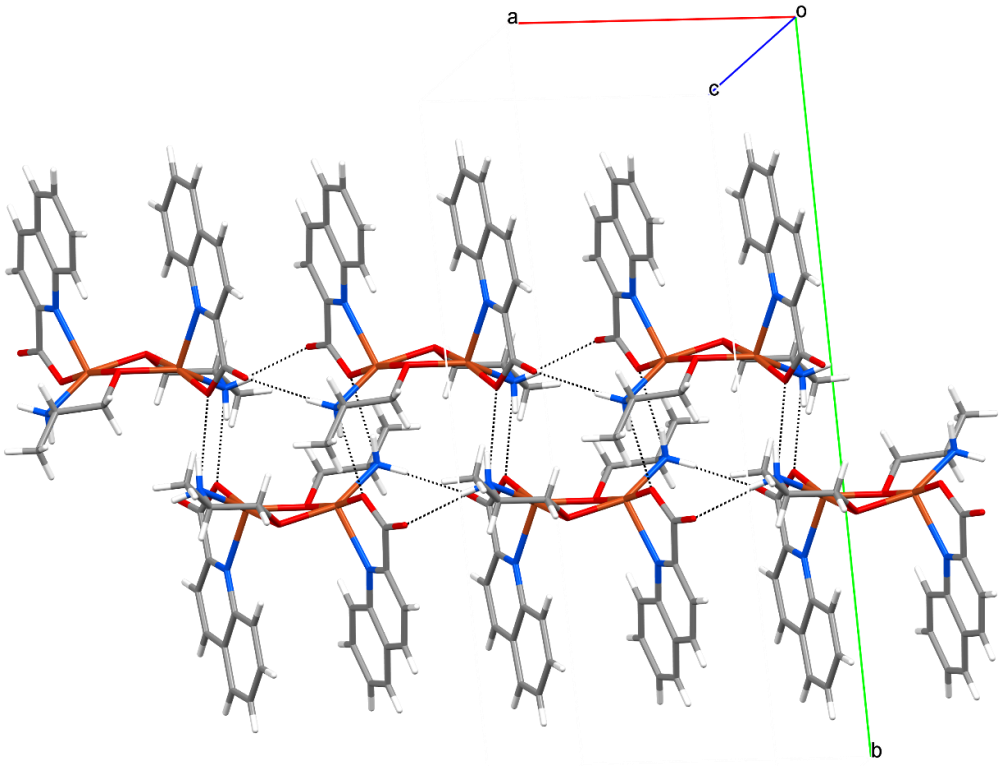


Figure S10. View of the supramolecular chain in ***syn*-11d**.

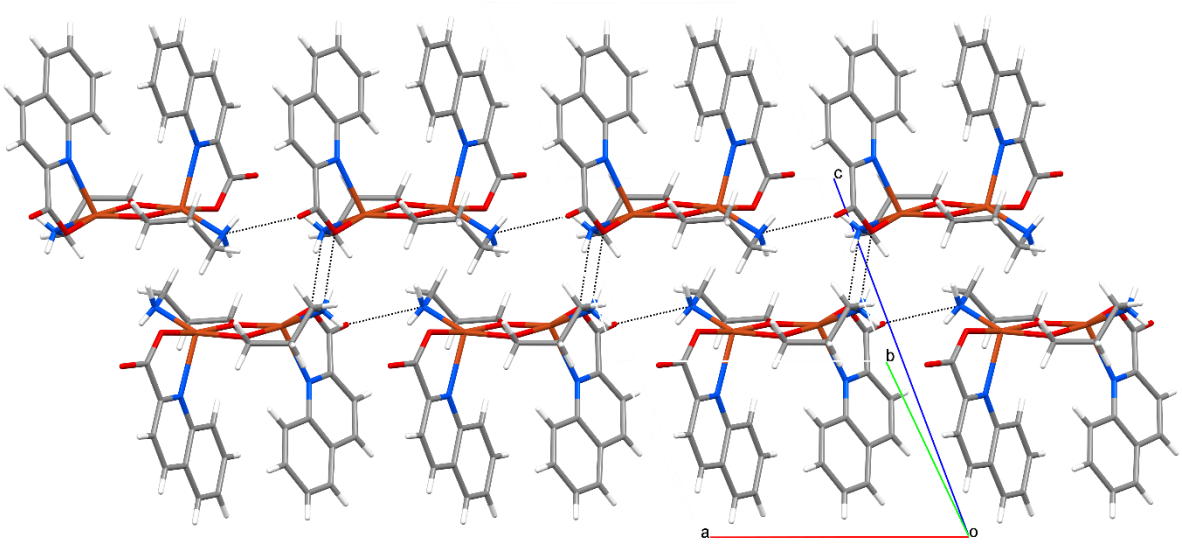


Figure S11. Structure of ***syn*-11d·2H₂O**: a perpendicular view to the supramolecular layer (top), and a view along the layer (bottom). The layers are coplanar with the *ab* plane and stack along *c*-axis. Colour code: light grey - dinuclear complex molecules, violet - water molecules.

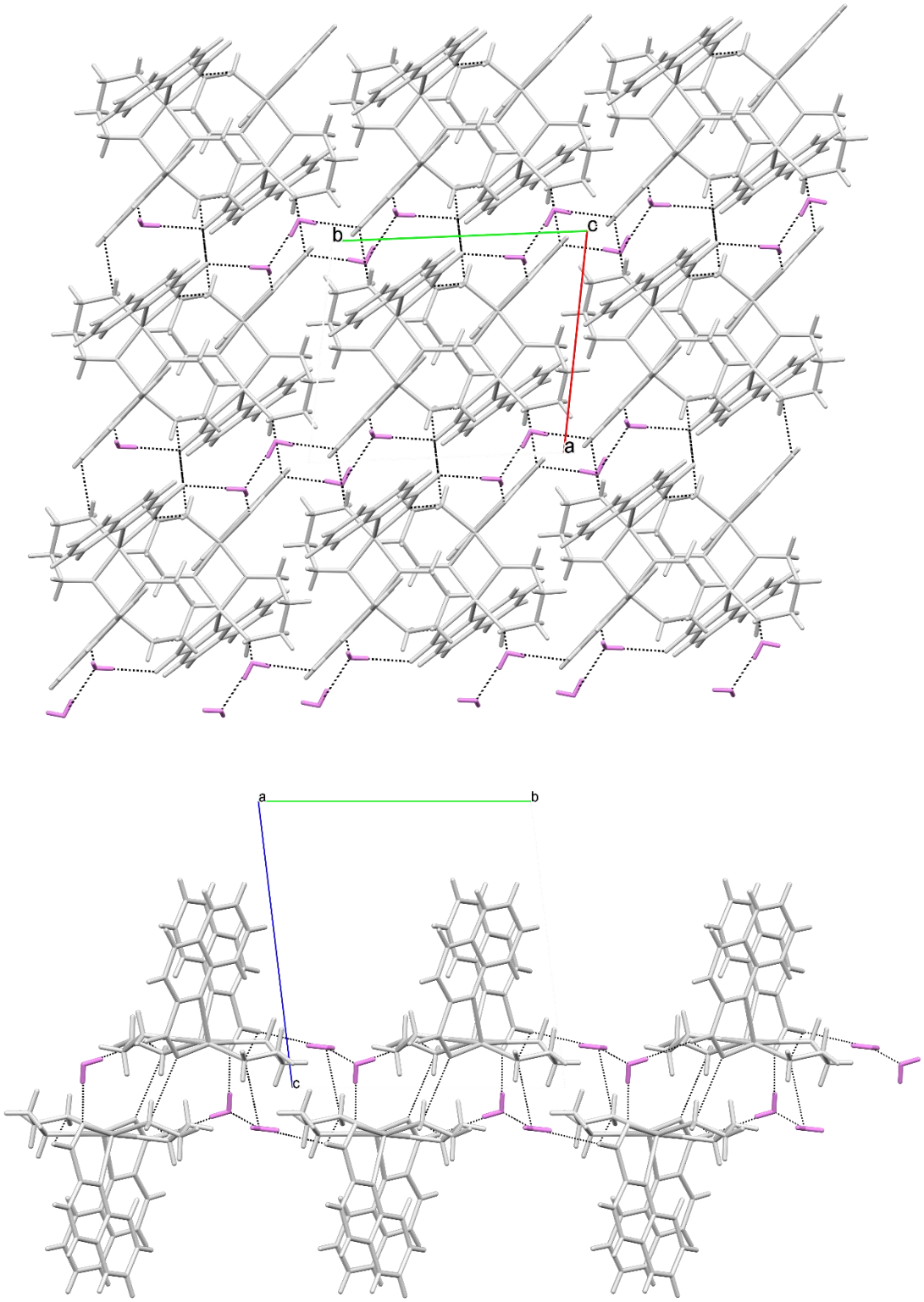
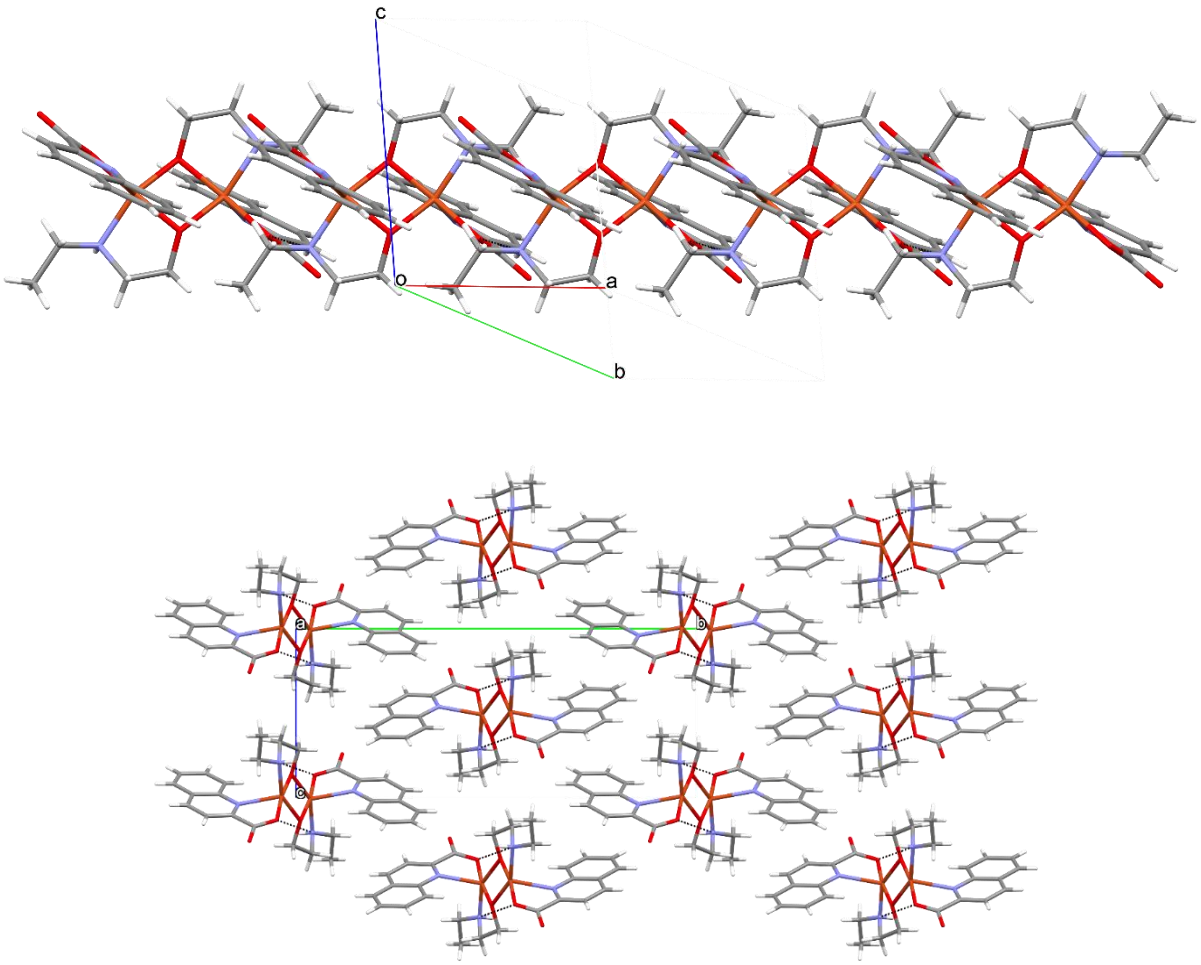


Figure S12. Structure of ***anti*-4d**: section of a chain of hydrogen bonded molecules (top), and a view along the chains (bottom). The connectivity may be described as $C_1^1(6)$ in graph set notation.[1]



[1] M. C. Etter, J. C. MacDonald and J. Bernstein, *Acta Crystallogr., Sect. B*, 1990, **46**, 256-262.

Figure S13. A view along the supramolecular layers in ***anti*-11d·2MeCN**. Acetonitrile molecules of crystallization (drawn in violet) are located in-between layers of complex molecules (light grey).

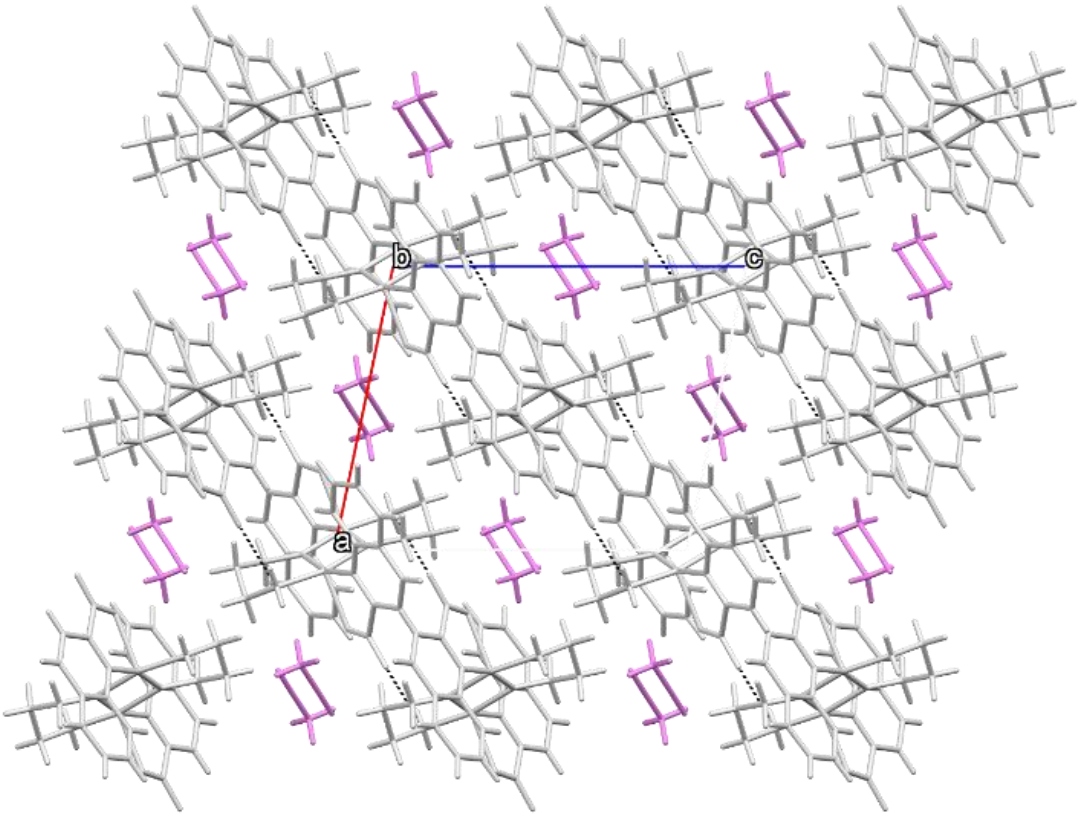


Figure S14. A view along the supramolecular layers in ***anti*-11d·4MeOH**. Colour code: light grey - complex molecules, violet - methanol molecules.

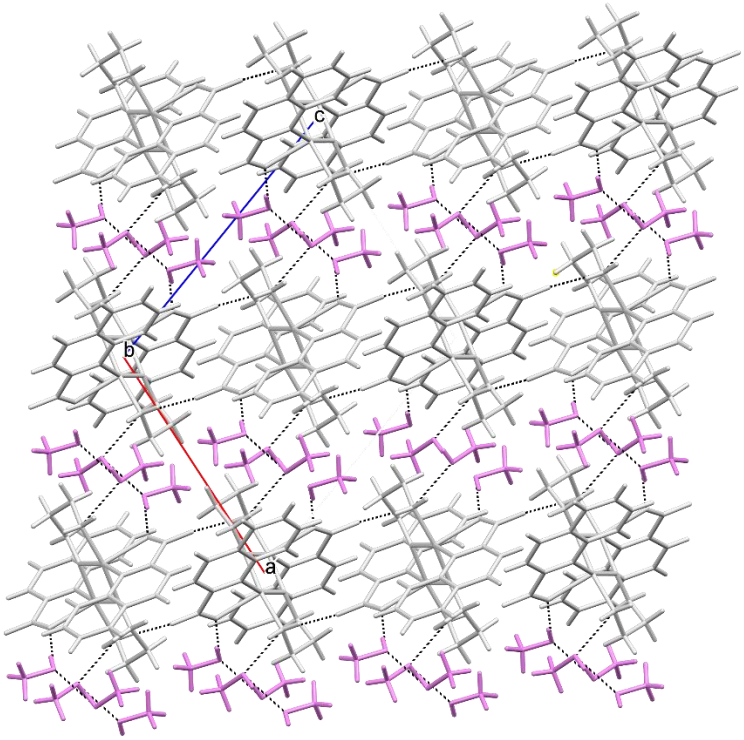


Figure S15. A view along the supramolecular layers in ***anti*-11d·2MeOH·2(3a1pOH)**. Colour code: light grey - complex molecules, violet - methanol molecules, light green - 3-amino-1-propanol molecules.

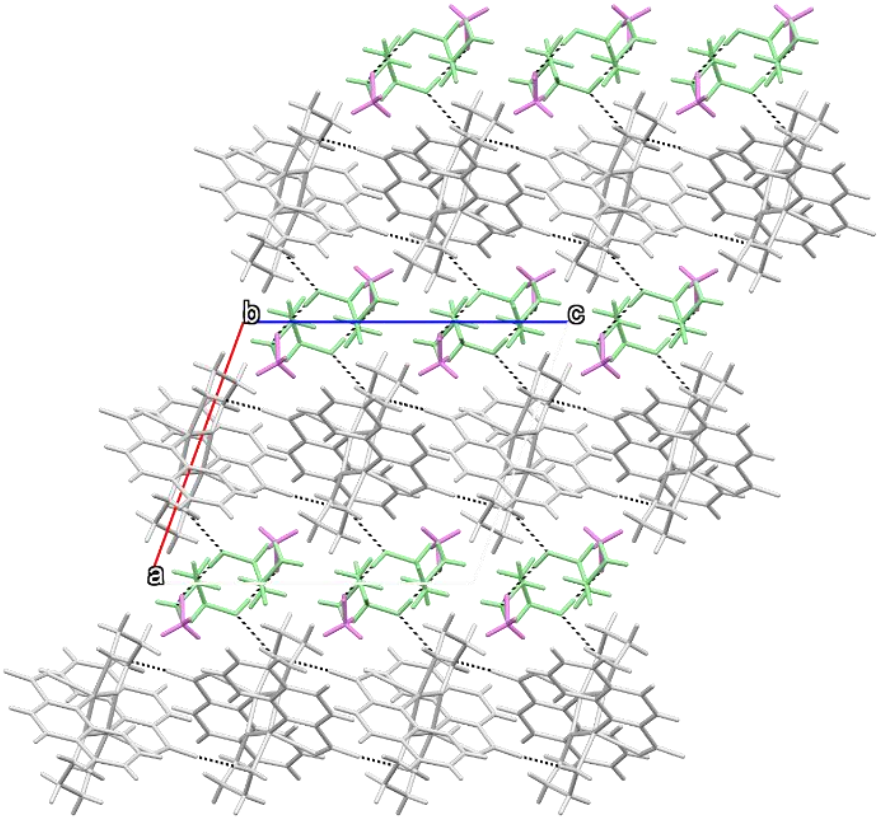


Figure S16. Section of a chain of hydrogen bonded complex cations and quinaldinate ions in **5e**.

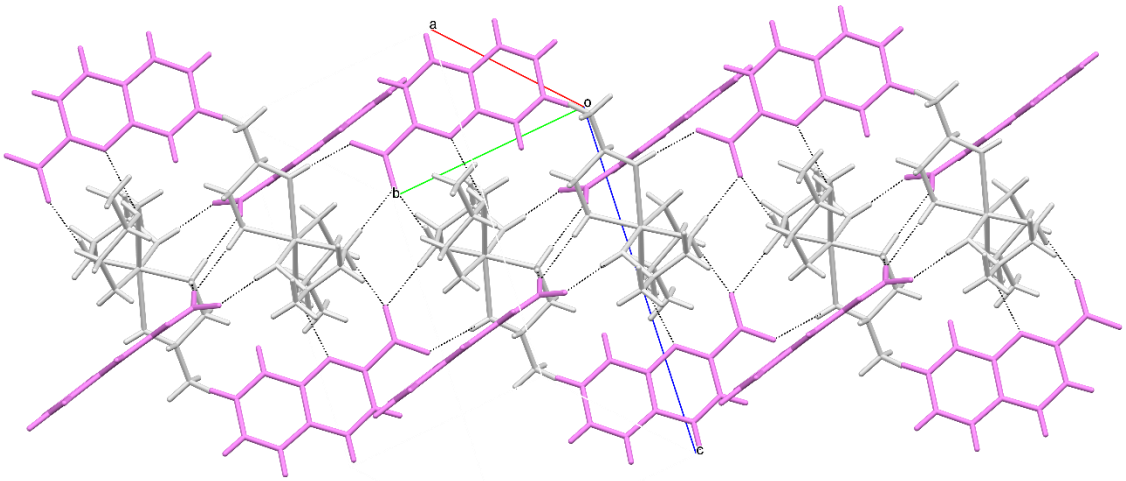


Figure S17. A view along the supramolecular chains in the structure of **7e**.

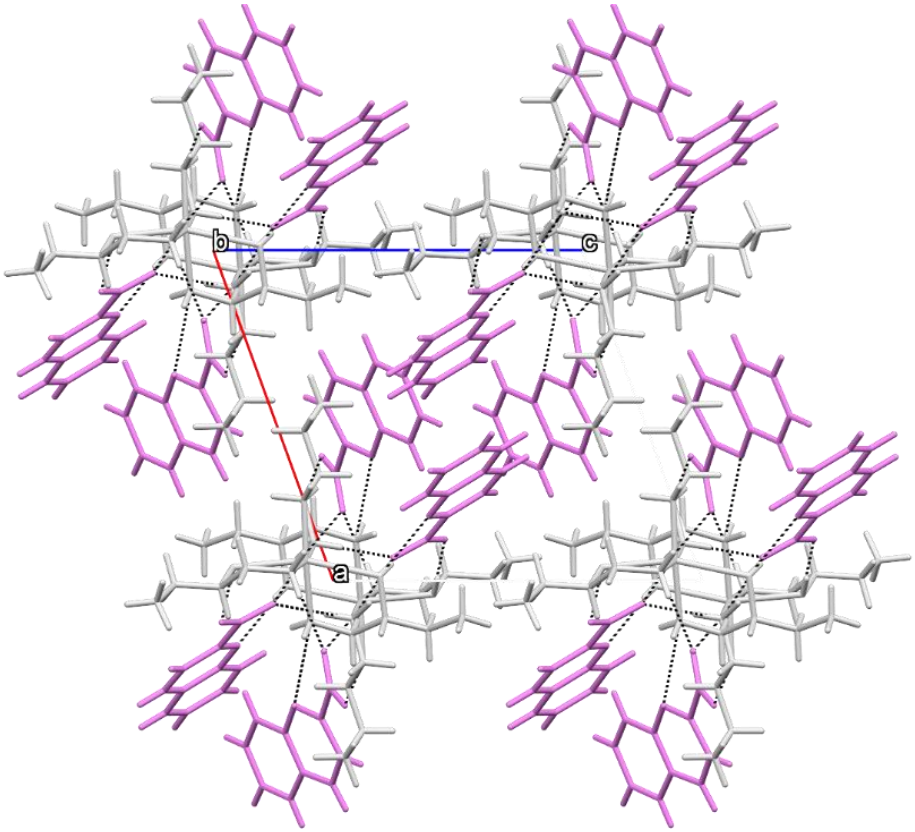


Figure S18. A perpendicular view to the supramolecular layer in **9f**. Colour code: light grey - complex molecules, pink - $(2a2m1pOHH)^+$ cations, and light green - $quin^-$ ions.

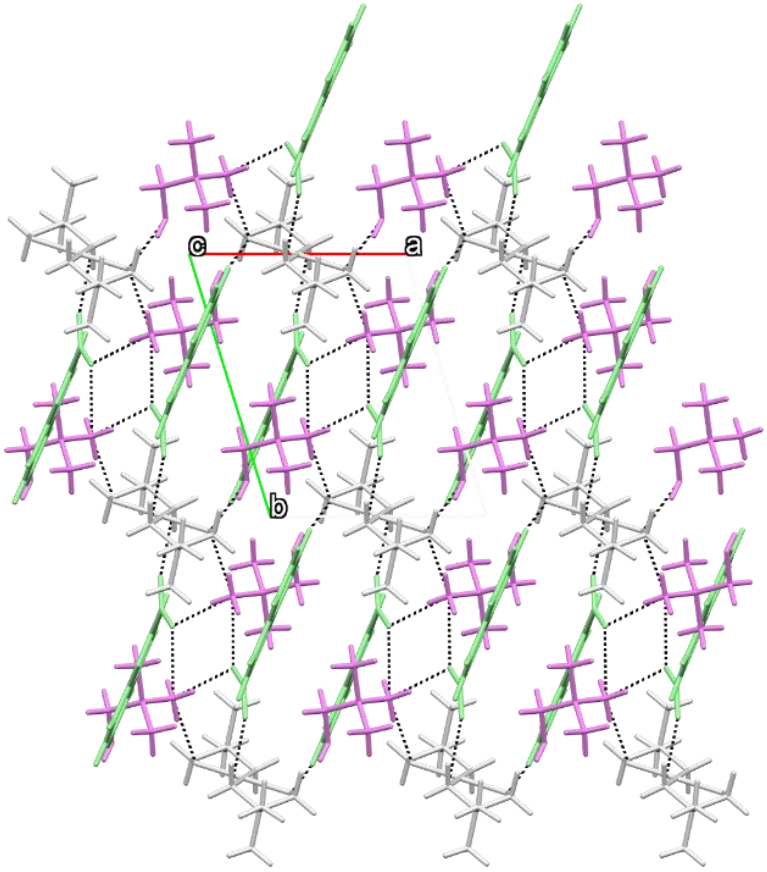


Figure S19. A view along the chains in the structure of **g**.

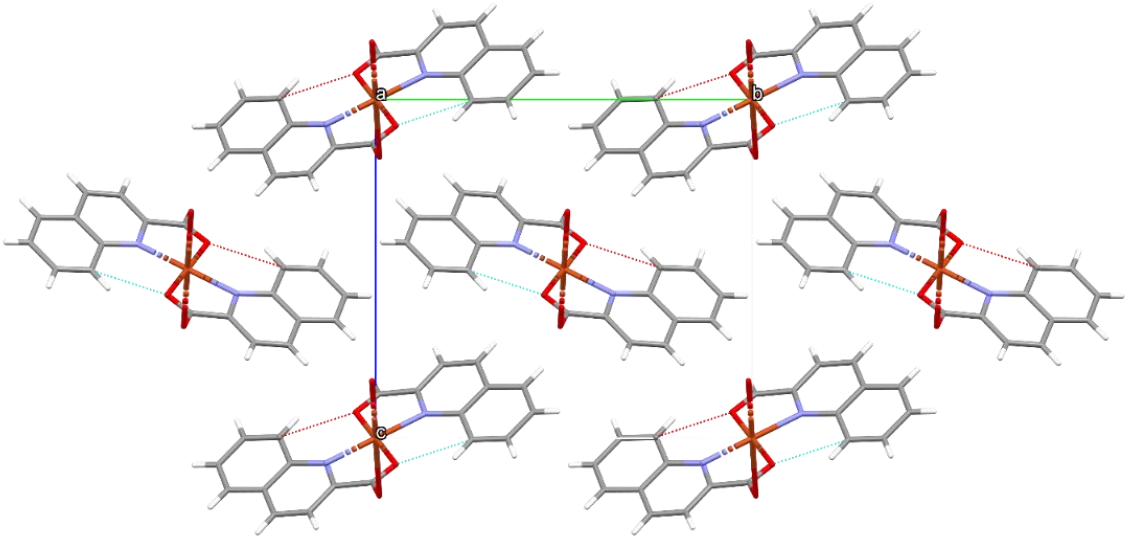


Table S4. Geometric parameters [Å, °] of type **d** complexes.

Compound	Amino alcohol	Cu–O$^-$	Cu···Cu	Planar/non-planar[a]	Cu–O(μ)–Cu	Deviation of the alkoxide carbon[b]
***syn*-8d**	2a1pOH	1.941(3), 1.974(3)	2.9177(9)	non-planar	96.36(13)	36.3(2)
***syn*-11d**	3a1pOH	1.9174(15)–1.9626(15)	3.0541(4)	planar	103.20(7), 104.62(7)	2.10(14), 3.40(14)
***syn*-11d·2H$_2$O**	3a1pOH	1.9275(16)–1.9432(17)	3.0433(4)	planar	103.25(8), 103.85(8)	3.99(16), 3.85(17)
***anti*-4d**	2eaeOH	1.929(2), 1.945(2)	2.9694(7)	planar	100.09(9)	38.0(2)
***anti*-11d·2MeCN**	3a1pOH	1.9270(12), 1.9459(12)	3.0433(5)	planar	103.58(5)	4.63(15)
***anti*-11d·4MeOH**	3a1pOH	1.9211(10), 1.9581(10)	3.0320(3)	planar	102.81(5)	20.89(12)
***anti*-11d·2MeOH·2(3a1pOH)**	3a1pOH	1.9353(10), 1.9518(10)	3.0530(3)	planar	103.52(5)	16.15(12)

[a] Refers to the Cu$_2$(μ-O)$_2$ unit.

[b] Given as a difference between 180° and the O(μ)–O(μ)–C angle.

Table S5. Hydrogen bonds [Å] in type **a** compounds.

1a	
OH···COO^-	O···O[*x*, 1+*y*, *z*] = 2.7742(19)
NH_2···COO^-	N···O[*x*, 1+*y*, *z*] = 3.036(2)
6a	
OH···COO^-	O···O[–1+*x*, *y*, *z*] = 2.772(2)
NH_2···COO^-	N···O[–1+*x*, *y*, *z*] = 3.009(2)
7a	
OH···COO^-	O···O[1+*x*, *y*, *z*] = 2.759(3)
OH···COO^-(coord.)[a]	O···O[1+*x*, *y*, *z*] = 2.973(5)
NH_2···COO^-	N···O[1+*x*, *y*, *z*] = 2.995(2)
11a	
OH···COO^-	O···O[1–*x*, 1–*y*, –*z*] = 2.7094(19)
11a·3a1pOH	
OH···COO^-	O···O = 2.684(2)
NH_2···COO^-	N···O[–1+*x*, *y*, *z*] = 2.968(2)
NH_2···COO^-	N···O[1+*x*, *y*, *z*] = 3.023(2)
NH_2···OH	N···O[1–*x*, 1–*y*, 1–*z*] = 2.981(2)
NH_2···OH(3a1pOH)[b]	N···O[1+*x*, *y*, *z*] = 3.037(2)
OH···NH_2(3a1pOH)[b]	O···N[1–*x*, 1–*y*, 1–*z*] = 2.820(3)
OH(3a1pOH)[b]···OH	O···O = 2.764(3)

[a] Carboxylate oxygen atom that is coordinated to copper(II) ion.

[b] Solvent molecules of 3-amino-1-propanol.

Table S6. Relevant intermolecular interactions [Å, °] in type **b** compounds.

2b	
***π*···*π* stacking interactions[a]**	
Ph···Ph type, *Cg*···*Cg* = 3.9175(9), interplanar angle = 0.02(8), shift distance = 1.693	
Hydrogen bonds	
OH···COO^-	O···O[*x*, 1–*y*, 0.5+*z*] = 2.792(3)
NH···COO^-	N···O[2–*x*, 1–*y*, –*z*] = 2.927(3)
8b	
***π*···*π* stacking interactions**	
Ph···Ph type, *Cg*···*Cg* = 3.8199(14), interplanar angle = 0.00(12), shift distance = 1.566	
Ph···Ph type, *Cg*···*Cg* = 3.9359(15), interplanar angle = 0.00(12), shift distance = 1.616	
Ph···Py type, *Cg*···*Cg* = 3.7389(13), interplanar angle = 2.43(11), shift distance = 1.456	
Ph···Py type, *Cg*···*Cg* = 3.7496(14), interplanar angle = 0.16(12), shift distance = 1.057	
Hydrogen bonds	
OH···COO^-	O···O[1–*x*, 1–*y*, –*z*] = 2.773(2)
NH_2···COO^-	N···O[1–*x*, 1–*y*, 1–*z*] = 2.933(2)
11b	
***π*···*π* stacking interactions**	
Ph···Ph type, *Cg*···*Cg* = 3.8858(13), interplanar angle = 0.02(10), shift distance = 1.481	
Ph···Py type, *Cg*···*Cg* = 3.7761(10), interplanar angle = 1.88(9), shift distance = 1.262	
Hydrogen bonds	
OH··· COO^-	O···O[0.5+*x*, 1–*y*, *z*] = 2.730(4)
NH_2···COO^-	N···O[1–*x*, 1–*y*, 1–*z*] = 2.967(4)

[a] Parameters as defined in C. Janiak, *J. Chem. Soc., Dalton Trans.* **2000**, 3885–3896.

Table S7. Relevant intermolecular interactions [Å, °] in type **c** compounds.

8c	
***π*···*π* stacking interactions**	
Ph···Ph type, *Cg*···*Cg* = 3.9190(15), interplanar angle = 0.03(12), shift distance = 1.889	
Ph···Py type, *Cg*···*Cg* = 3.7104(15), interplanar angle = 0.72(12), shift distance = 1.393	
Hydrogen bonds	
OH···COO^-	O···O[0.5+*x*, 0.5–*y*, 0.5+*z*] = 2.684(4)
NH_2···COO^-	N···O[0.5–*x*, –0.5+*y*, 0.5–*z*] = 2.907(5)
11c	
***π*···*π* stacking interactions**	
Ph···Py type, *Cg*···*Cg* = 3.9521(13), interplanar angle = 2.44(11), shift distance = 1.715	
Hydrogen bonds	
OH···COO^-	O···O[1.5–*x*,0.5+*y*,1.5–*z*] = 2.646(6)
NH_2···COO^-	N···O[–0.5+*x*, 0.5–*y*, –0.5+*z*] = 2.835(6)

Table S8. Relevant intra- and intermolecular interactions [Å, °] in *syn*-$[Cu_2(quin)_2(OR)_2]$ compounds.

***syn*-8d**	
$\pi\cdots\pi$ stacking interactions	
intramolecular, Ph···Ph type, *Cg*···*Cg* = 3.926(2), interplanar angle = 11.1(2), shift distance = 1.760	
intermolecular, Py···Py type, *Cg*···*Cg* = 3.650(2), interplanar angle = 8.2(2), shift distance = 1.439	
Hydrogen bonds	
$NH_2\cdots COO^-$	N···O[0.5–*x*, *y*, 1–*z*] = 2.954(4)
$NH_2\cdots COO^-$(coord.)[a]	N···O[1–*x*, 1–*y*, 1–*z*] = 2.978(5)
***syn*-11d**	
$\pi\cdots\pi$ stacking interactions	
intramolecular, Ph···Ph type, *Cg*···*Cg* = 3.7534(17), interplanar angle = 14.76(13), shift distance = 1.711	
Hydrogen bonds	
$NH_2\cdots COO^-$	N···O[–1+*x*, *y*, *z*] = 3.002(3)
$NH_2\cdots COO^-$(coord.)[a]	N···O[2–*x*, 1–*y*, 1–*z*] = 3.025(3)
***syn*-11d·2H_2O**	
$\pi\cdots\pi$ stacking interactions	
intermolecular, Py···Py type, *Cg*···*Cg* = 3.9019(15), interplanar angle = 12.39(12), shift distance = 1.930	
Hydrogen bonds	
$NH_2\cdots COO^-$(coord.)[a]	N···O[1–*x*, 1–*y*, 2–*z*] = 3.013(3)
$NH_2\cdots COO^-$	N···O[1+*x*, *y*, *z*] = 2.949(3)
$NH_2\cdots COO^-$	N···O[–1+*x*, *y*, *z*] = 2.973(3)
$NH_2\cdots H_2O$	N···O[–*x*, 1–*y*, 2–*z*] = 3.031(4)
$H_2O\cdots COO^-$	O···O[–1+*x*, –1+*y*, *z*] = 2.890(3)
$H_2O\cdots COO^-$	O···O = 2.806(3)
$H_2O\cdots COO^-$(coord.)[a]	O···O[1–*x*, 1–*y*, 2–*z*] = 2.858(3)
$H_2O\cdots H_2O$	O···O = 2.797(3)

[a] Carboxylate oxygen atom that is coordinated to copper(II) ion.

Table S9. Relevant intermolecular interactions [Å, °] in the structures of *anti*-$[Cu_2(quin)_2(OR)_2]$ compounds.

***anti*-4d**	
$\pi\cdots\pi$ stacking interactions	
Ph···Py type, *Cg*···*Cg* = 3.7248(18), interplanar angle = 14.96(15), shift distance = 1.498	
Hydrogen bonds	
NH···COO^-(coord.)[a]	N···O[–*x*, 1–*y*, 1–*z*] = 2.924(3)
***anti*-11d·2MeCN**	
$\pi\cdots\pi$ stacking interactions	
Ph···Ph type, *Cg*···*Cg* = 3.6881(11), interplanar angle = 0.02(9), shift distance = 1.358	
Ph···Py type, *Cg*···*Cg* = 3.7716(10), interplanar angle = 2.77(8), shift distance = 1.674	
Hydrogen bonds	
NH_2···COO^-	N···O[–0.5+*x*, 1.5–*y*, –0.5+*z*] = 2.9172(19)
***anti*-11d·4MeOH**	
$\pi\cdots\pi$ stacking interactions	
Ph···Ph type, *Cg*···*Cg* = 3.8249(10), interplanar angle = 0.02(9), shift distance = 1.774	
Ph···Py type, *Cg*···*Cg* = 3.7853(9), interplanar angle = 0.31(8), shift distance = 1.687	
Hydrogen bonds	
NH_2···COO^-	N···O[0.5+*x*, 1.5–*y*, 0.5+*z*] = 2.8964(18)
NH_2···MeOH	N···O[1.5–*x*, 0.5+*y*, 0.5–*z*] = 3.0221(19)
MeOH···COO^-(coord.)[a]	O···O = 2.7843(18)
MeOH···MeOH	O···O = 2.795(2)
***anti*-11d·2MeOH·2(3a1pOH)**	
$\pi\cdots\pi$ stacking interactions	
Ph···Ph type, *Cg*···*Cg* = 3.7971(10), interplanar angle = 0.00(8), shift distance = 1.706	
Ph···Py type, *Cg*···*Cg* = 3.7136(9), interplanar angle = 1.83(8), shift distance = 1.584	
Hydrogen bonds	
NH_2···COO^-	N···O[*x*, 0.5–*y*, –0.5+*z*] = 2.8982(18)
NH_2···OH(3a1pOH)	N···O = 2.9837(18)
MeOH···NH_2(3a1pOH)	N···O = 2.657(2)
OH(3a1pOH)···MeOH	O···O[2–*x*, –0.5+*y*, 1.5–*z*] = 2.708(2)

[a] Carboxylate oxygen atom that is coordinated to copper(II) ion.

Table S10. Relevant intermolecular interactions [Å, °] in type **e** compounds.

5e	
***π*···*π* stacking interactions**	
Ph···Ph type, *Cg*···*Cg* = 3.7477(16), interplanar angle = 0.00(13), shift distance = 1.635	
Hydrogen bonds	
OH···COO^-	O···O = 2.548(3)
OH···COO^-	O···O = 2.681(3)
OH···N($quin^-$)	O···N[2–*x*, 1–*y*, 1–*z*] = 2.837(3)
NH_2···COO^-	N···O[1–*x*, –*y*, 1–*z*] = 2.894(3)
NH_2···COO^-	N···O = 2.981(3)
NH_2···COO^-	N···O = 2.923(3)
NH_2···COO^-	N···O[2–*x*, 1–*y*, 1–*z*] = 2.908(3)

7e	
***π*···*π* stacking interaction**	
Ph···Ph type, *Cg*···*Cg* = 3.7052(15), interplanar angle = 0.00(12), shift distance = 1.666	
Hydrogen bonds	
OH···COO^-	O···O = 2.710(3)
OH···COO^-	O···O = 2.529(3)
OH···N($quin^-$)	O···N[1–*x*, 1–*y*, 1–*z*] = 2.832(3)
NH_2···COO^-	N···O = 3.040(3)
NH_2···COO^-	N···O[1–*x*, 2–*y*, 1–*z*] = 2.904(3)
NH_2···COO^-	N···O = 2.883(3)
NH_2···COO^-	N···O[1–*x*, 1–*y*, 1–*z*] = 2.889(3)
NH_2···N($quin^-$)	N···N[1–*x*, 2–*y*, 1–*z*] = 3.046(3)

8e	
***π*···*π* stacking interaction**	
Ph···Ph type, *Cg*···*Cg* = 3.782(7), interplanar angle = 6.2(6), shift distance = 1.398	
Ph···Ph type, *Cg*···*Cg* = 3.695(8), interplanar angle = 2.4(7), shift distance = 1.445	
Ph···Ph type, *Cg*···*Cg* = 3.959(6), interplanar angle = 4.3(5), shift distance = 1.543	
Hydrogen bonds	
OH···COO^-	O···O = 2.610(5)
OH···COO^-	O···O = 2.656(6)
OH···COO^-	O···O[–1+*x*, 1+*y*, *z*] = 2.975(9)
OH···COO^-	O···O[–1+*x*, 1+*y*, *z*] = 2.497(10)
OH···COO^-	O···O = 2.582(13)
OH···COO^-	O···O = 2.571(8)
OH···COO^-	O···O = 2.406(16)
OH···COO^-	O···O = 2.614(11)
OH···N($quin^-$)	O···N = 2.914(8)
NH_2···COO^-	N···O[–1+*x*, 1+*y*, *z*] = 2.977(7)
NH_2···COO^-	N···O[–1+*x*, 1+*y*, *z*] = 2.906(6)
NH_2···COO^-	N···O = 2.924(5)
NH_2···COO^-	N···O = 2.685(12)
NH_2···COO^-	N···O = 2.860(12)
NH_2···COO^-	N···O = 2.924(15)

Table S11. Relevant intermolecular interactions [Å, °] in type **e** compounds, continuation.

10e	
***π*···*π* stacking interactions**	
Ph···Py type, *Cg*···*Cg* = 3.906(3), interplanar angle = 1.6(2), shift distance = 2.014	
Py···Py type, *Cg*···*Cg* = 3.480(2), interplanar angle = 0.0(2), shift distance = 0.943	
Hydrogen bonds	
OH···COO^-	O···O = 2.685(4)
OH···COO^-	O···O = 2.508(4)
OH···COO^-	O···O = 2.760(4)
OH···COO^-	O···O = 2.490(4)
OH···COO^-	O···O = 2.723(4)
OH···COO^-	O···O = 2.742(4)
OH···COO^-	O···O = 2.518(4)
OH···COO^-	O···O = 2.729(4)
OH···COO^-	O···O[1–*x*, 1–*y*, 1–*z*] = 2.757(4)
OH···COO^-	O···O = 2.695(4)
OH···COO^-	O···O = 2.521(4)
OH···COO^-	O···O[–1–*x*, 2–*y*, 2–*z*] = 2.761(4)
NH_2···COO^-	N···O = 3.063(4)
NH_2···COO^-	N···O = 3.007(4)
NH_2···COO^-	N···O = 3.061(4)
NH_2···COO^-	N···O[1+*x*, *y*, *z*] = 2.998(4)
NH_2···COO^-	N···O = 3.051(4)
NH_2···COO^-	N···O = 3.019(5)
NH_2···COO^-	N···O = 2.986(4)
NH_2···COO^-	N···O = 3.014(5)
NH_2···COO^-	N···O[–*x*, 1–*y*, 1–*z*] = 3.035(5)
NH_2···COO^-	N···O = 2.996(4)
NH_2···COO^-	N···O[–1–*x*, 2–*y*, 2–*z*] = 2.967(4)
NH_2···COO^-	N···O = 3.056(4)
NH_2···COO^-	N···O[–*x*, 2–*y*, 2–*z*] = 3.035(4)
NH_2···N($quin^-$)	N···N[1+*x*, *y*, *z*] = 3.091(5)
NH_2···N($quin^-$)	N···N[–*x*, 2–*y*, 2–*z*] = 3.039(4)

Table S12. Relevant intermolecular interactions [Å, °] in **9f**.

9f	
***π*···*π* stacking interactions**	
Ph···Py type, *Cg*···*Cg* = 3.9871(11), interplanar angle = 1.53(10), shift distance = 1.628	
Hydrogen bonds	
OH···O(coordinated amino alcoholate)	O···O = 2.6606(16)
NH_2···COO^-	N···O[–1+*x*, *y*, *z*] = 2.8603(18)
NH_3^+···O(coordinated amino alcoholate)	N···O[–*x*, 2–*y*, 2–*z*] = 2.7909(17)
NH_3^+···COO^-	N···O = 2.8149(18)
NH_3^+···COO^-	N···O[1–*x*, 1–*y*, 2–*z*] = 2.8570(18)

Table S13. Relevant intra- and intermolecular interactions [Å, °] in **g**.

g	
***π*···*π* stacking interactions**	
Ph···Py type, *Cg*···*Cg* = 3.8273(9), interplanar angle = 2.91(7), shift distance = 1.703	
Short intramolecular contact	
C–H···COO^-(coord.)[a]	C···O[1–*x*, 1–*y*, 1–*z*] = 2.9530(18)

[a] Carboxylate oxygen atom that is coordinated to copper(II) ion.

Table S14. Shortest Cu···Cu contacts.[a]

Compound	Hydrogen bonded motif	Cu···Cu[Å]
1a	chains	5.9728(2)
6a	chains	6.0630(3)
7a	chains	5.8410(3)
11a	chains	5.6066(3)[b]
11a·3a1pOH	3D-network	7.4853(3)
2b	chains	7.0950(2)[c]
8b	chains	6.8047(6)
11b	chains	7.0537(2)
8c	layers	7.6001(4)
11c	layers	7.5417(4)
***syn*-8d**	chains	2.9177(9)
***syn*-11d**	chains	3.0541(4)
***syn*-11d·2H$_2$O**	layers	3.0433(4)
***anti*-4d**	chains	2.9694(7)
***anti*-11d·2MeCN**	layers	3.0433(5)
***anti*-11d·4MeOH**	3D-network	3.0320(3)
***anti*-11d·2MeOH·2(3a1pOH)**	3D-network	3.0530(3)
5e	chains	6.6225(8)
7e	chains	6.5514(6)
8e	chains	6.8633(7)
10e	chains	7.0937(9)
9f	layers	8.1133(4)
g	/	4.8617(2)[d]

[a] The shortest contact, if not stated otherwise, occurs within the hydrogen bonded motif. For type **d** compounds, the shortest contact occurs within the dinuclear moiety.

[b] The pair of metal ions belongs to adjacent chains. The shortest distance within the chain is much longer, 11.2830(7) Å.

[c] The average distance.

[d] Occurs between copper(II) ions that are bridged with a pair of quinaldinates.

3. DFT calculations

Table S15. Zero-Point and free energy changes for the interconversion of **11a**, **11a–L** and **11b**.

	ΔZPE	ΔG
11a → 11a–L + 3a1pOH	5.46	–2.88
11a–L → 11b	0.14	2.08
11a → 11b + 3a1pOH	5.60	–0.80

Table S16. Comparison of the experimentally determined and calculated bond lengths [Å] for **11a** and **11b**.

	X-ray	**Calculated**
11a		
Cu–NH_2	2.0184(14)	2.027, 2.028
Cu–N(quin$^-$)	2.4185(14)	2.333, 2.353
Cu–O(quin$^-$)	2.0034(11)	2.052, 2.055
11b		
Cu–NH_2	1.953(4)	2.024
Cu–OH	2.510(4)	2.437
Cu–N(quin$^-$)	2.2408(13)	2.077, 2.505
Cu–O(quin$^-$)	1.9468(11)	1.972, 1.985

Table S17. Correlation of the magnetic coupling constants with the $Cu_2(\mu\text{-}O)_2$ bridge geometry for optimized *syn*- and *anti*-$[Cu_2(quin)_2(3a1pO)_2]$.

	θ [°]	τ [°]	$-2J$ [K][a]
syn-$[Cu_2(quin)_2(3a1pO)_2]$	97.8	43	–163.1
anti-$[Cu_2(quin)_2(3a1pO)_2]$	100.4	28	–494.6

[a] L. J. Farrugia, D. S. Middlemiss, R. Sillanpää and P. Seppälä, *J. Phys. Chem. A*, 2008, **112**, 9050–9067.

3. 1. Lists of optimized geometries

14
3a1pOH; E = -249.663680222 a.u.

N	-1.396844000	-0.852416000	-0.057441000
H	-2.159403000	-1.226694000	0.500829000
H	-1.672436000	-0.958062000	-1.031558000
C	-1.184367000	0.573764000	0.251300000
H	-2.014167000	1.205256000	-0.098463000
H	-1.140532000	0.671440000	1.342730000
C	0.132249000	1.061244000	-0.348914000
C	1.344690000	0.331022000	0.219110000
O	1.328915000	-1.063924000	-0.069201000
H	0.377598000	-1.318943000	-0.004214000
H	2.269055000	0.742512000	-0.203566000
H	1.383572000	0.493602000	1.309903000
H	0.239852000	2.134651000	-0.148071000
H	0.107620000	0.938360000	-1.440877000

67
11a; E = -1876.36675797 a.u.

Cu	0.093636000	0.055695000	0.008281000
O	-0.026820000	0.954952000	1.848619000
O	-1.337443000	1.691877000	3.511114000
N	0.277772000	-1.688107000	1.027551000
N	-2.190861000	0.080700000	0.481951000
C	-1.159563000	1.144196000	2.410000000
C	-4.590075000	-0.240108000	0.246162000
C	-3.681072000	0.821701000	2.212974000
C	-2.391280000	0.651602000	1.655728000
C	-3.252679000	-0.370532000	-0.238899000
C	-4.081484000	-1.443174000	-2.240505000
C	-3.018204000	-0.980839000	-1.496783000
C	-4.773524000	0.376604000	1.508122000
C	-5.409997000	-1.316715000	-1.764047000
C	-5.661166000	-0.726860000	-0.544750000
O	0.429166000	-6.554626000	1.363142000
C	0.291622000	-2.961785000	0.293567000
C	0.356081000	-4.171814000	1.217400000
C	0.366479000	-5.471179000	0.435674000
H	1.130860000	-1.598977000	1.578125000
H	-0.606611000	-2.996402000	-0.329290000
H	1.233462000	-5.495353000	-0.240842000
H	1.151850000	-2.950891000	-0.380752000
H	-5.779806000	0.490600000	1.903462000
H	1.260939000	-4.114859000	1.836421000
H	-0.541743000	-5.546246000	-0.180228000
H	-6.677255000	-0.626179000	-0.171903000
H	-0.507749000	-4.164081000	1.894933000
H	-0.487124000	-1.692543000	1.700679000
H	-1.992137000	-1.068004000	-1.845505000
H	-3.903117000	-1.911690000	-3.204626000
H	-3.776008000	1.300420000	3.180477000
H	0.433101000	-7.379923000	0.861755000
H	-6.232918000	-1.688895000	-2.367820000
O	0.219648000	-0.818206000	-1.847806000
O	1.519155000	-1.574464000	-3.510174000
N	-0.052795000	1.803173000	-1.009073000
N	2.399129000	-0.038831000	-0.450601000
C	1.350539000	-1.046645000	-2.397851000
C	4.807701000	0.133435000	-0.157356000
C	3.881922000	-0.885600000	-2.139078000
C	2.591882000	-0.631321000	-1.614465000
C	3.469584000	0.351337000	0.292939000
C	4.313623000	1.385316000	2.308521000
C	3.242312000	0.984933000	1.540636000
C	4.982734000	-0.504213000	-1.410272000
C	5.642944000	1.172451000	1.866343000
C	5.887067000	0.558532000	0.657438000
O	-1.125119000	6.541424000	-1.485898000
C	-0.536861000	3.018774000	-0.339182000
C	-0.590987000	4.223197000	-1.271169000
C	-1.099270000	5.459421000	-0.554968000
H	-0.648662000	1.587061000	-1.806982000
H	0.120746000	3.213826000	0.511630000
H	-2.107169000	5.273836000	-0.155415000
H	-1.531797000	2.804224000	0.060970000
H	5.989196000	-0.684071000	-1.779885000
H	-1.248877000	4.001572000	-2.121654000
H	-0.441276000	5.699400000	0.293104000
H	6.903976000	0.392009000	0.311331000
H	0.410783000	4.423552000	-1.673031000
H	0.875217000	1.972016000	-1.395252000
H	2.215281000	1.137529000	1.863256000
H	4.141159000	1.870924000	3.265216000
H	3.970078000	-1.376123000	-3.101367000
H	-1.446984000	7.326768000	-1.025258000
H	6.472354000	1.497036000	2.488425000

53
11a–L; E = -1626.69348186 a.u.

Cu	-1.203234000	-2.337667000	0.915123000
O	-1.055066000	-1.779453000	2.791112000
O	-0.894788000	0.062375000	4.064120000
N	-0.557660000	-4.154914000	1.474657000
N	-1.849132000	-0.358459000	0.708677000
C	-1.081185000	-0.505843000	2.984420000
C	-1.827260000	1.692437000	-0.587488000
C	-1.104611000	1.698203000	1.712052000
C	-1.377303000	0.317569000	1.749339000
C	-2.154351000	0.310527000	-0.443650000
C	-3.027221000	0.286055000	-2.696581000
C	-2.785473000	-0.370145000	-1.509658000
C	-1.282535000	2.371859000	0.528433000
C	-2.649193000	1.638259000	-2.866917000
C	-2.068393000	2.331777000	-1.828492000
O	3.330879000	-7.025391000	2.179332000
C	0.908994000	-4.274470000	1.394324000
C	1.415481000	-5.641179000	1.836911000
C	2.927523000	-5.725349000	1.750476000
H	-0.866822000	-4.334232000	2.429103000
H	1.200033000	-4.067736000	0.360624000
H	3.383264000	-4.953063000	2.387328000
H	1.338807000	-3.484602000	2.017641000
H	-1.022376000	3.422726000	0.436241000
H	1.100639000	-5.833448000	2.870637000
H	3.255019000	-5.544019000	0.716306000
H	-1.797637000	3.378553000	-1.936650000
H	0.971672000	-6.420957000	1.204765000
H	-0.994634000	-4.855541000	0.877894000
H	-3.063292000	-1.408731000	-1.373899000
H	-3.508460000	-0.242995000	-3.513982000
H	-0.713400000	2.178837000	2.600627000
H	4.293889000	-7.074717000	2.124549000
H	-2.832767000	2.131703000	-3.816869000
O	-1.393646000	-3.063413000	-0.912101000
O	-0.696704000	-3.030761000	-3.040521000
N	0.624216000	-1.347511000	-0.280729000
C	-0.674787000	-2.607103000	-1.878381000
C	1.603870000	0.821463000	-0.784394000
C	0.522230000	-0.461179000	-2.517260000
C	0.229177000	-1.438402000	-1.538083000
C	1.342563000	-0.259173000	0.110742000
C	2.426571000	0.957649000	1.898573000
C	1.782009000	-0.175521000	1.453828000
C	1.178218000	0.681472000	-2.128653000
C	2.657222000	2.045718000	1.023339000
C	2.259542000	1.977995000	-0.294584000
H	1.367625000	1.486153000	-2.834102000
H	2.443095000	2.804684000	-0.976025000
H	1.585563000	-1.013224000	2.115706000
H	2.750772000	1.024474000	2.933159000
H	0.175970000	-0.607552000	-3.533609000
H	3.154921000	2.936368000	1.396132000

53
11b; E = -1626.69412165 a.u.

C	0.740457000	2.060865000	-3.573793000
C	-0.486602000	1.379540000	-3.396824000
C	1.486622000	2.440799000	-2.480437000
C	-0.936261000	1.050810000	-2.137095000
C	-0.949946000	-2.025022000	-1.694711000
C	1.469840000	-1.405551000	-2.119723000
C	1.041835000	2.136422000	-1.170187000
C	-0.167086000	1.396227000	-1.002227000
C	0.440774000	-1.695667000	-1.192929000
C	2.662736000	-0.917999000	-1.645765000
C	1.744855000	2.543133000	-0.011144000
C	-4.729362000	-0.721045000	0.323469000
C	2.854692000	-0.780228000	-0.248705000
C	1.240163000	2.238755000	1.229340000
C	0.081765000	1.442871000	1.309867000
C	1.789468000	-1.186082000	0.611038000
C	4.039101000	-0.252405000	0.321906000
C	-5.011600000	-1.563393000	1.562961000
C	-0.461592000	0.981914000	2.645387000
C	1.953844000	-1.093005000	2.014256000
C	-3.793694000	-1.853235000	2.435179000
C	4.165706000	-0.150155000	1.690520000
C	3.120198000	-0.582641000	2.540590000
H	1.084485000	2.295225000	-4.576966000
H	-1.078483000	1.107636000	-4.266073000
H	2.418331000	2.986879000	-2.601003000
H	1.276689000	-1.520502000	-3.179880000
H	-1.869948000	0.520624000	-1.991512000
H	3.458829000	-0.624586000	-2.324952000
H	2.670905000	3.101016000	-0.119490000
H	-4.233528000	-1.318550000	-0.444884000
H	-5.673196000	-0.348151000	-0.094764000
H	4.841145000	0.068607000	-0.337872000
H	-2.851186000	-2.934544000	0.937029000
H	-4.144216000	0.878710000	1.323010000
H	-5.464961000	-2.502848000	1.221425000
H	1.727499000	2.546976000	2.146494000
H	-1.919728000	-2.679238000	2.254828000
H	-5.756318000	-1.065959000	2.196330000
H	1.136419000	-1.414142000	2.652513000
H	-4.046756000	-2.642501000	3.152568000
H	5.072752000	0.261524000	2.123860000
H	-3.511266000	-0.966576000	3.007963000
H	3.236170000	-0.498227000	3.617403000
Cu	-1.648149000	-0.689670000	0.770986000
N	-0.576529000	1.009105000	0.242079000
N	0.590775000	-1.602345000	0.116096000
N	-2.608541000	-2.242865000	1.644862000
O	-1.071760000	-2.625161000	-2.771142000
O	-1.924967000	-1.618550000	-0.961490000
O	-3.832500000	0.369937000	0.562049000
O	-1.331995000	0.038206000	2.576460000
O	-0.063263000	1.523194000	3.682381000

66
singlet_anti_11d; E = -2072.61960828 a.u.

Cu	-1.743425000	10.706547000	12.076029000
O	0.257174000	10.630932000	13.148430000
C	-2.914609000	8.105871000	12.956753000
N	-1.838592000	8.937403000	13.059921000
C	0.352182000	9.619226000	13.900278000
O	1.294273000	9.317969000	14.663981000
C	-5.070541000	7.616806000	11.981887000
H	-5.884566000	7.878886000	11.312162000
C	-0.827946000	8.639783000	13.861200000
C	-4.128547000	6.077837000	13.601097000
H	-4.179955000	5.166231000	14.190467000
C	-3.974472000	8.444085000	12.082304000
H	-3.902159000	9.361185000	11.503161000
C	-5.150468000	6.427095000	12.746365000
H	-6.024902000	5.789487000	12.654068000
C	-0.826682000	7.466646000	14.648180000
H	0.027278000	7.276033000	15.287219000
C	-1.899890000	6.610747000	14.584786000
H	-1.928585000	5.704193000	15.183813000
C	-2.986290000	6.908002000	13.726402000
O	-2.055968000	12.367710000	11.121865000
N	-0.906304000	9.837702000	10.443678000
C	0.015162000	10.699717000	9.678406000
H	0.440707000	10.135436000	8.839021000
H	0.836462000	10.974096000	10.348545000
C	-0.683920000	11.948781000	9.164236000
H	-1.568613000	11.661577000	8.579062000
H	-0.000081000	12.466936000	8.480108000
C	-1.097889000	12.923200000	10.259779000
H	-0.199494000	13.241272000	10.818027000
H	-1.514285000	13.823306000	9.785504000
H	-1.651687000	9.507160000	9.831753000
H	-0.412678000	9.008284000	10.767199000
Cu	-3.170036000	13.325463000	12.434702000
O	-5.190172000	13.137049000	11.402543000
C	-2.290805000	15.979486000	11.393171000
N	-3.262708000	15.024161000	11.340217000
C	-5.347643000	14.038386000	10.530484000
O	-6.267696000	14.141146000	9.691021000
C	-0.221513000	16.779061000	12.349873000
H	0.606133000	16.659076000	13.043080000
C	-4.286495000	15.146085000	10.509859000
C	-1.310023000	18.088204000	10.623814000
H	-1.354923000	18.958451000	9.974470000
C	-1.212454000	15.824586000	12.295809000
H	-1.189847000	14.946119000	12.935950000
C	-0.268252000	17.917511000	11.508452000
H	0.524745000	18.657593000	11.565376000
C	-4.408425000	16.254191000	9.642067000
H	-5.265923000	16.298414000	8.981204000
C	-3.444945000	17.233800000	9.658743000
H	-3.511379000	18.095719000	8.999747000
C	-2.346286000	17.124060000	10.545367000
O	-2.778529000	11.702453000	13.423660000
N	-4.013958000	14.222222000	14.045642000
C	-4.867250000	13.351892000	14.877491000
H	-5.290703000	13.931068000	15.707694000
H	-5.696166000	13.010945000	14.248627000
C	-4.092054000	12.159333000	15.415755000
H	-3.198334000	12.510404000	15.950191000
H	-4.723629000	11.643735000	16.150205000
C	-3.682738000	11.153729000	14.347306000
H	-4.589431000	10.779560000	13.840719000
H	-3.214489000	10.290951000	14.842385000
H	-3.270651000	14.618932000	14.619708000
H	-4.558865000	15.009674000	13.700220000

66
triplet_anti_11d; E = -2072.61804261 a.u.

Cu	-1.957503000	10.723457000	11.952408000
O	0.099769000	10.894951000	12.896281000
C	-2.799222000	8.053847000	13.012843000
N	-1.832031000	9.014672000	13.036578000
C	0.266281000	10.016078000	13.789627000
O	1.193651000	9.936694000	14.623436000
C	-4.884125000	7.235717000	12.106823000
H	-5.727207000	7.345671000	11.430766000
C	-0.790000000	8.905146000	13.845441000
C	-3.751507000	5.946192000	13.819478000
H	-3.688236000	5.081525000	14.474728000
C	-3.897566000	8.195771000	12.132422000
H	-3.938084000	9.070373000	11.488089000
C	-4.812768000	6.104134000	12.955853000
H	-5.602629000	5.359289000	12.921820000
C	-0.643719000	7.805712000	14.720647000
H	0.227650000	7.772094000	15.363794000
C	-1.601476000	6.820367000	14.732559000
H	-1.516090000	5.964468000	15.397193000
C	-2.719114000	6.916380000	13.868319000
O	-2.356421000	12.339155000	10.950516000
N	-1.186334000	9.817870000	10.303822000
C	-0.255210000	10.663155000	9.531289000
H	0.153440000	10.093771000	8.686925000
H	0.573990000	10.922127000	10.197453000
C	-0.937066000	11.925517000	9.026037000
H	-1.816643000	11.655148000	8.425311000
H	-0.239496000	12.446352000	8.357979000
C	-1.357850000	12.890013000	10.127054000
H	-0.469956000	13.178728000	10.714978000
H	-1.743289000	13.807062000	9.658865000
H	-1.952888000	9.515904000	9.703509000
H	-0.710584000	8.971448000	10.609314000
Cu	-3.284064000	13.325110000	12.382488000
O	-5.311074000	13.410178000	11.362821000
C	-2.145263000	15.946033000	11.491189000
N	-3.209868000	15.100207000	11.394748000
C	-5.381605000	14.371763000	10.545225000
O	-6.292984000	14.614839000	9.725475000
C	-0.006490000	16.478461000	12.480074000
H	0.802814000	16.239819000	13.164124000
C	-4.213483000	15.365939000	10.574077000
C	-0.946839000	17.973144000	10.818035000
H	-0.898007000	18.872663000	10.210119000
C	-1.092250000	15.637224000	12.384309000
H	-1.164000000	14.730224000	12.979720000
C	0.068606000	17.653091000	11.691877000
H	0.934756000	18.302394000	11.780797000
C	-4.218148000	16.520151000	9.759279000
H	-5.064847000	16.684550000	9.103486000
C	-3.157211000	17.391766000	9.818199000
H	-3.132291000	18.285039000	9.199336000
C	-2.078307000	17.127754000	10.696814000
O	-2.942510000	11.683019000	13.364657000
N	-4.086755000	14.198346000	14.033382000
C	-5.059586000	13.352150000	14.751689000
H	-5.486916000	13.908282000	15.595652000
H	-5.870675000	13.127159000	14.051532000
C	-4.420326000	12.064228000	15.248602000
H	-3.559069000	12.302586000	15.888158000
H	-5.151705000	11.539675000	15.876375000
C	-3.973883000	11.121973000	14.138322000
H	-4.844813000	10.858056000	13.513427000
H	-3.615048000	10.188563000	14.595397000
H	-3.334685000	14.469273000	14.665967000
H	-4.535996000	15.061158000	13.733731000

66
singlet_syn_11d; E = -2072.63032736 a.u.

Cu	0.317733000	1.234342000	2.153626000
Cu	3.258048000	1.057292000	1.873365000
O	1.730792000	1.989128000	1.034444000
O	1.831949000	0.221638000	2.912269000
O	-1.009438000	0.379857000	3.377947000
O	-1.905907000	0.410518000	5.430834000
O	4.599177000	2.010428000	0.743397000
O	5.734530000	3.921578000	0.465283000
N	0.069628000	2.820483000	3.769577000
N	3.942136000	2.721835000	3.262232000
N	-1.148946000	2.009619000	0.998310000
H	-2.012348000	1.526934000	1.240111000
H	-1.266635000	2.974456000	1.305270000
N	4.640937000	-0.295173000	2.461502000
H	5.417826000	-0.235320000	1.805861000
H	4.998444000	0.041924000	3.354877000
C	-0.664518000	2.315186000	4.743172000
C	-0.929447000	3.017680000	5.941339000
H	-1.530271000	2.543106000	6.708382000
C	-0.412964000	4.282456000	6.097127000
H	-0.591327000	4.851034000	7.006403000
C	0.362416000	4.856732000	5.061349000
C	0.924448000	6.156085000	5.135252000
H	0.760648000	6.748478000	6.031786000
C	1.665338000	6.650966000	4.085114000
H	2.096682000	7.646213000	4.146306000
C	1.883942000	5.865737000	2.926061000
H	2.484086000	6.268383000	2.115124000
C	1.362223000	4.596359000	2.826735000
H	1.544333000	3.952883000	1.969307000
C	0.587045000	4.071842000	3.890793000
C	4.706703000	3.549311000	2.573847000
C	5.209428000	4.753989000	3.117203000
H	5.824535000	5.395107000	2.496582000
C	4.897164000	5.077165000	4.416533000
H	5.259858000	5.997833000	4.866715000
C	4.089217000	4.203173000	5.182529000
C	3.720697000	4.459474000	6.527210000
H	4.069661000	5.372810000	7.002094000
C	2.930767000	3.562870000	7.211700000
H	2.646502000	3.764353000	8.240751000
C	2.468995000	2.382397000	6.578702000
H	1.833119000	1.695893000	7.130404000
C	2.799692000	2.108452000	5.271357000
H	2.427430000	1.234022000	4.743245000
C	3.620539000	3.011830000	4.551475000
C	-0.935101000	1.977872000	-0.461218000
H	-0.897848000	0.926406000	-0.767139000
H	-1.785293000	2.444627000	-0.974304000
C	0.357225000	2.679902000	-0.851234000
H	0.347354000	3.710107000	-0.469657000
H	0.393531000	2.743876000	-1.946028000
C	1.617765000	1.972691000	-0.369293000
H	1.616733000	0.937121000	-0.755271000
H	2.498591000	2.472900000	-0.796110000
C	1.729504000	-1.179025000	3.016858000
H	1.487048000	-1.633001000	2.038966000
H	0.898551000	-1.417497000	3.695595000
C	3.009664000	-1.810638000	3.549147000
H	3.264253000	-1.361561000	4.519012000
H	2.820015000	-2.876238000	3.729262000
C	4.196196000	-1.694671000	2.603837000
H	5.026060000	-2.315498000	2.964040000
H	3.917986000	-2.055681000	1.607456000
C	-1.239100000	0.921997000	4.516611000
C	5.042517000	3.145045000	1.143333000

66
triplet_syn_11d; E = -2072.62980868 a.u.

Cu	0.345258000	1.254563000	2.195628000
Cu	3.251736000	1.097200000	1.907307000
O	1.729098000	2.021818000	1.048464000
O	1.852538000	0.226682000	2.955277000
O	-0.979015000	0.390385000	3.423790000
O	-1.874720000	0.426758000	5.477380000
O	4.589433000	2.052607000	0.767053000
O	5.716165000	3.969169000	0.487445000
N	0.084029000	2.839165000	3.799356000
N	3.936557000	2.756846000	3.287518000
N	-1.139047000	1.997958000	1.035436000
H	-2.004772000	1.545802000	1.323246000
H	-1.232875000	2.981713000	1.284954000
N	4.646667000	-0.259857000	2.470300000
H	5.447666000	-0.141834000	1.852816000
H	4.959670000	0.016754000	3.400256000
C	-0.646005000	2.334816000	4.776846000
C	-0.914028000	3.042288000	5.971128000
H	-1.511336000	2.568088000	6.741113000
C	-0.403951000	4.310377000	6.120074000
H	-0.583593000	4.882398000	7.026925000
C	0.366205000	4.883861000	5.080054000
C	0.920982000	6.186665000	5.147413000
H	0.756024000	6.781507000	6.042102000
C	1.656064000	6.681700000	4.093348000
H	2.082053000	7.679545000	4.149358000
C	1.874564000	5.893579000	2.936316000
H	2.468768000	6.296911000	2.121359000
C	1.359813000	4.620822000	2.843219000
H	1.540846000	3.977973000	1.985020000
C	0.592582000	4.095138000	3.912395000
C	4.695612000	3.588912000	2.598077000
C	5.193926000	4.795119000	3.141484000
H	5.804623000	5.439456000	2.519868000
C	4.881965000	5.116347000	4.441276000
H	5.240085000	6.038959000	4.891123000
C	4.080407000	4.237594000	5.208408000
C	3.712927000	4.492263000	6.553650000
H	4.057029000	5.408104000	7.027237000
C	2.930287000	3.590928000	7.240180000
H	2.646476000	3.791074000	8.269605000
C	2.476337000	2.406526000	6.608994000
H	1.847410000	1.715256000	7.162699000
C	2.806337000	2.133788000	5.301138000
H	2.441368000	1.253437000	4.777595000
C	3.617761000	3.043320000	4.578408000
C	-0.952951000	1.872222000	-0.422734000
H	-0.927760000	0.803025000	-0.661382000
H	-1.808661000	2.311620000	-0.950719000
C	0.337277000	2.538029000	-0.878689000
H	0.331788000	3.596042000	-0.582575000
H	0.365152000	2.511935000	-1.975285000
C	1.601239000	1.873641000	-0.348462000
H	1.594515000	0.806852000	-0.635904000
H	2.479136000	2.329552000	-0.827462000
C	1.743917000	-1.179047000	2.900274000
H	1.527293000	-1.520214000	1.872027000
H	0.893717000	-1.485018000	3.525777000
C	3.007790000	-1.870319000	3.394711000
H	3.240865000	-1.520046000	4.409643000
H	2.808889000	-2.947096000	3.464873000
C	4.217281000	-1.671087000	2.493204000
H	5.044268000	-2.310301000	2.827159000
H	3.969368000	-1.957225000	1.464961000
C	-1.211757000	0.936702000	4.559251000
C	5.029226000	3.188345000	1.166057000

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singlet_anti_11d opt without empirical dispersion; E = -2072.43565354 a.u.

Cu	-1.773242000	10.666747000	12.118858000
O	0.182679000	10.627012000	13.244797000
C	-2.902239000	7.991622000	13.018717000
N	-1.864489000	8.873338000	13.139931000
C	0.316143000	9.604762000	13.977319000
O	1.267970000	9.327013000	14.737369000
C	-5.047505000	7.431709000	12.048028000
H	-5.885651000	7.683350000	11.403776000
C	-0.827532000	8.581865000	13.912723000
C	-3.995098000	5.864781000	13.568336000
H	-3.986766000	4.921534000	14.108885000
C	-3.997224000	8.313872000	12.180003000
H	-3.986753000	9.264135000	11.651726000
C	-5.048624000	6.199138000	12.746055000
H	-5.886783000	5.517622000	12.629548000
C	-0.756554000	7.374271000	14.644854000
H	0.116557000	7.197202000	15.262288000
C	-1.783729000	6.466341000	14.551689000
H	-1.754287000	5.529265000	15.102551000
C	-2.898104000	6.750701000	13.724422000
O	-2.016101000	12.341615000	11.139002000
N	-0.961240000	9.738076000	10.482664000
C	-0.084269000	10.549671000	9.612750000
H	0.261414000	9.940649000	8.767290000
H	0.796449000	10.829472000	10.200823000
C	-0.791268000	11.796113000	9.101235000
H	-1.719058000	11.511393000	8.585150000
H	-0.143486000	12.271848000	8.353147000
C	-1.102924000	12.823025000	10.186164000
H	-0.155909000	13.131210000	10.665924000
H	-1.520501000	13.718577000	9.703422000
H	-1.734547000	9.370707000	9.928079000
H	-0.446558000	8.925694000	10.817779000
Cu	-3.202653000	13.366768000	12.356295000
O	-5.148235000	13.233270000	11.203215000
C	-2.262541000	16.087773000	11.386656000
N	-3.218873000	15.118286000	11.264778000
C	-5.286410000	14.167619000	10.362560000
O	-6.185318000	14.299908000	9.504781000
C	-0.236001000	16.881607000	12.445293000
H	0.573014000	16.742547000	13.157368000
C	-4.226150000	15.277161000	10.417525000
C	-1.302819000	18.256215000	10.757889000
H	-1.348248000	19.159016000	10.153829000
C	-1.204802000	15.910938000	12.311740000
H	-1.183821000	15.001557000	12.907854000
C	-0.282519000	18.061592000	11.662925000
H	0.492035000	18.814306000	11.781625000
C	-4.343056000	16.426627000	9.602320000
H	-5.187012000	16.493794000	8.925483000
C	-3.395361000	17.417578000	9.691343000
H	-3.461289000	18.312236000	9.076716000
C	-2.316925000	17.276908000	10.599063000
O	-2.891289000	11.725449000	13.370938000
N	-4.079817000	14.305784000	13.951285000
C	-4.884590000	13.478393000	14.873768000
H	-5.253563000	14.100368000	15.699684000
H	-5.756010000	13.115353000	14.318202000
C	-4.085769000	12.304674000	15.420358000
H	-3.161468000	12.670155000	15.889785000
H	-4.678298000	11.827854000	16.212203000
C	-3.748479000	11.245100000	14.375747000
H	-4.691261000	10.863165000	13.943909000
H	-3.266574000	10.398961000	14.887041000
H	-3.333803000	14.761954000	14.476610000
H	-4.657615000	15.056353000	13.577150000

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singlet_syn_11d opt without empirical dispersion; E = -2072.43543360 a.u.

Cu	0.286953000	1.258881000	2.134028000
Cu	3.279843000	1.027447000	1.873634000
O	1.758562000	2.073757000	1.129524000
O	1.824520000	0.315537000	2.974351000
O	-1.089690000	0.262063000	3.185003000
O	-2.491942000	0.186800000	4.928783000
O	4.632252000	1.790137000	0.614395000
O	6.253852000	3.281243000	0.214262000
N	-0.423709000	2.817434000	3.784770000
N	4.425231000	2.649781000	3.174734000
N	-1.163039000	1.938414000	0.868670000
H	-1.961114000	1.314786000	0.979031000
H	-1.459714000	2.841036000	1.238122000
N	4.611794000	-0.414591000	2.417405000
H	5.297535000	-0.477094000	1.666517000
H	5.113246000	-0.040941000	3.222722000
C	-1.337960000	2.225979000	4.533401000
C	-2.016589000	2.886791000	5.586535000
H	-2.752085000	2.337836000	6.163716000
C	-1.728068000	4.206351000	5.839686000
H	-2.232926000	4.747223000	6.636797000
C	-0.762085000	4.875746000	5.047709000
C	-0.413618000	6.238706000	5.231780000
H	-0.905305000	6.804895000	6.019304000
C	0.532098000	6.829431000	4.422148000
H	0.795128000	7.874129000	4.565472000
C	1.168958000	6.082450000	3.399880000
H	1.914685000	6.564082000	2.772546000
C	0.854422000	4.756449000	3.196731000
H	1.335318000	4.162557000	2.422757000
C	-0.119260000	4.126464000	4.013825000
C	5.338108000	3.216406000	2.405628000
C	6.229241000	4.212857000	2.874253000
H	6.951394000	4.637830000	2.186271000
C	6.155976000	4.606408000	4.188922000
H	6.826943000	5.365438000	4.584617000
C	5.194205000	4.013341000	5.044352000
C	5.055094000	4.354789000	6.414420000
H	5.714843000	5.108600000	6.837624000
C	4.097761000	3.738117000	7.190354000
H	3.994600000	4.002223000	8.239521000
C	3.240331000	2.759439000	6.628598000
H	2.487819000	2.286686000	7.254609000
C	3.348914000	2.406329000	5.301165000
H	2.695284000	1.665228000	4.846378000
C	4.329932000	3.022935000	4.482560000
C	-0.824382000	2.082725000	-0.561115000
H	-0.667013000	1.077892000	-0.969260000
H	-1.668951000	2.530818000	-1.100401000
C	0.427358000	2.926664000	-0.752516000
H	0.300419000	3.898246000	-0.255097000
H	0.539326000	3.133047000	-1.825005000
C	1.710659000	2.257440000	-0.271225000
H	1.819635000	1.292054000	-0.797733000
H	2.567046000	2.877588000	-0.570466000
C	1.693742000	-1.057027000	3.282197000
H	1.347772000	-1.626127000	2.400526000
H	0.919357000	-1.169650000	4.053628000
C	2.987031000	-1.688534000	3.787477000
H	3.346108000	-1.150354000	4.675716000
H	2.756706000	-2.712468000	4.109685000
C	4.093673000	-1.757969000	2.745202000
H	4.912584000	-2.394550000	3.104376000
H	3.711034000	-2.202305000	1.819425000
C	-1.672305000	0.774729000	4.204544000
C	5.422982000	2.737473000	0.959897000

4. Infrared spectroscopy

Table S18. Frequencies [cm^{-1}] in the carboxylate signature regions.[a]

	$\nu_{as}(COO^-)$	$\nu_{s}(COO^-)$
Monodentate coordination of carboxylate		
1a	1604vs, 1587vs	1372vs, 1345s
6a	1609s, 1587s	1369s, 1336s
7a	1594s	1370s, 1343s
11a	1623s	1371vs, 1342s
11a·3a1pOH	1614s	1377s, 1359s
2b	1640s	1362vs, 1343s
8b	1641s	1361vs, 1342s
11b	1641s	1362vs, 1342s
8c	1641s, 1624s	1359s, 1341s
11c	1644s, 1628s	1360vs, 1343s
***anti*-4d**	1636vvs	1360vs
***anti*-11d·2MeCN**	1630vs	1359vs, 1343s
***anti*-11d·4MeOH**	1632s	1359s, 1342s
***anti*-11d·2MeOH·2(3a1pOH)**	1628vs	1365vs, 1343s
***syn*-8d**	1635vvs	1352vs
***syn*-9d**	1638vvs	1361vs
***syn*-10d**	1636vvs	1351vs
***syn*-11d·2H_2O**	1633vs, 1615vs	1372vs, 1343s
Bidentate bridging coordination of carboxylate		
g	1637s	1372s, 1357s
Ionic carboxylate		
5e	1553s	1369vs, 1341s
7e	1550s	1367vs, 1340s
8e	1557s	1365vs, 1337s
10e	1557s	1366vs, 1337s
9f	1553s	1372vs

[a] Tentative assignations.

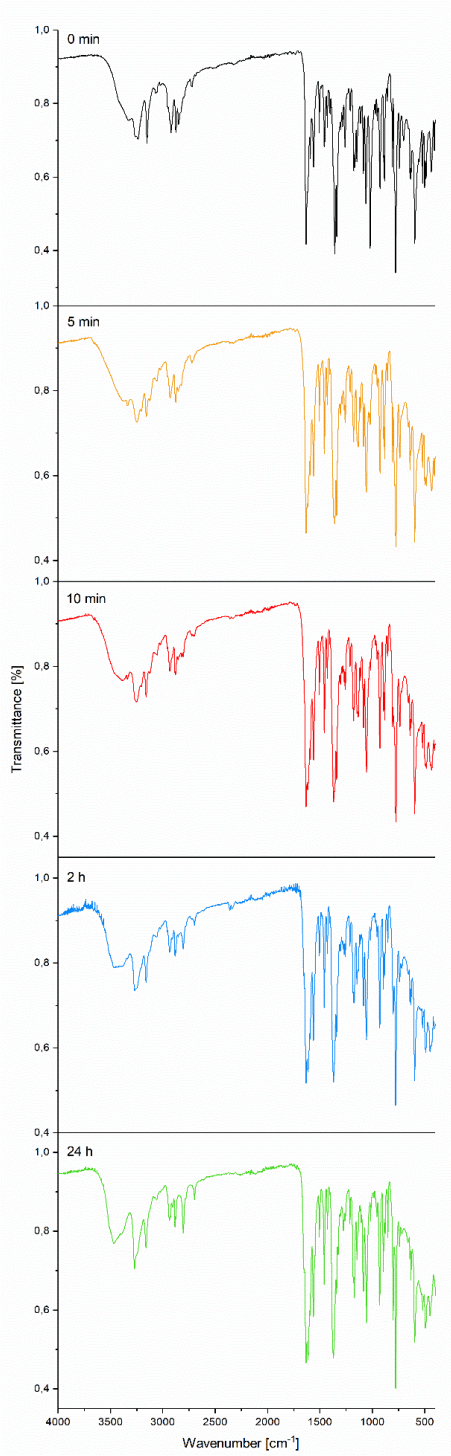
Table S19. Relevant IR absorptions [cm^{-1}] of the amino alcohol/alcoholate in Cu(II) compounds.

	***ν*(N–H)/*ν*(O–H) region**	***ν*(C–O)**	**out-of-plane C–OH**
Monodentate coordination of amino alcohol *via* NH_2			
1a	3284s broad, 3156w	1034vvs	708s broad
6a	3323m, 3244w, 3148w	1178–958 (several bands, s, m)	672m broad
7a	3260m, 3166w	1137–961 (several bands, s, m)	707m broad
11a	3384m, 3329m, 3224m	1051s, 1030m, 1021m	not observed
11a·3a1pOH	3359w, 3255m, 3175m	1060s, 1044s, 1017m	672m broad
Bidentate chelating coordination of amino alcohol			
2b	3378w, 3211m	1058m, 1029s	662m broad
8b	3376w, 3343w, 3226w, 3140w	1053s, 1039s	678m broad
11b	3345m, 3233m, 3154m	1046m	661s
5e	3236m, 3122m	1117–1026 (several, s)	707m broad
7e	3263m, 3212m, 3139m	1110–955 (several, s, m)	700m broad
8e	3213m, 3123m	1043s	680m broad
10e	3218m, 3125m	1044vs	not observed
Bidentate bridging coordination of amino alcohol			
8c	3302w, 3214w, 3133w	1076s, 1060s	not observed
11c	3335w, 3238w, 3154w	1066s, 1034m	not observed
Tridentate bridging coordination of amino alcoholate[a]			
***anti*-4d**	3183m	1062s, 1032s	–
***anti*-11d·2MeCN**	3310m, 3219w, 3141w	1082s, 1059s	–
***anti*-11d·4MeOH**	3332–3151 (several, m)	1063s, 1022vs	–
***anti*-11d·2MeOH·2(3a1pOH)**	3386–3152 (several, m)	1051s	–
***syn*-8d**	3323w, 3251s, 3145m	1070s, 1047s	–
***syn*-9d**	3255m, 3145m	1068m, 1047s, 1019m	–
***syn*-10d**	3255s, 3143m	1075s	–
***syn*-11d·2H_2O**	3271m, 3160m	1085s, 1055s	–
Bidentate chelating coordination of amino alcoholate, protonated amino alcohol as counterion[b]			
9f	3315m, 3200–2500m very broad	1055vvs, 1010s	690m

[a] Please see Section 3. 2. in the manuscript for the exact description of the amino alcoholate coordination mode.

[b] **9f** contains two forms of amino alcohol: the alcoholate that is bound to copper(II) and the cationic form with NH_3^+ moiety.

Figure S20. A time evolution of the IR spectra of ***anti*-11d·4MeOH** at room temperature. The conversion into ***syn*-11d·2H₂O** is completed within 24 hours. Color code: *t* = 0 min (black curve), 5 min (orange), 10 min (red), 2 h (blue) and 24 h (green).



With time, the spectrum undergoes major changes. The most apparent ones pertain to the methanol and water absorption bands. A very intense absorption band at 1022 cm^{-1} which originates in the ν(C–O) vibration of methanol rapidly loses intensity. Within the first five minutes, its intensity is reduced to *ca*. one third of the initial value. The 3469 cm^{-1} spectral region features a slow appearance of a new peak which can be attributed to the ν(O–H) water vibration.

Figure S21. Infrared spectrum of *trans*-[Cu(quin)$_2$(2aeOH)$_2$] (**1a**).

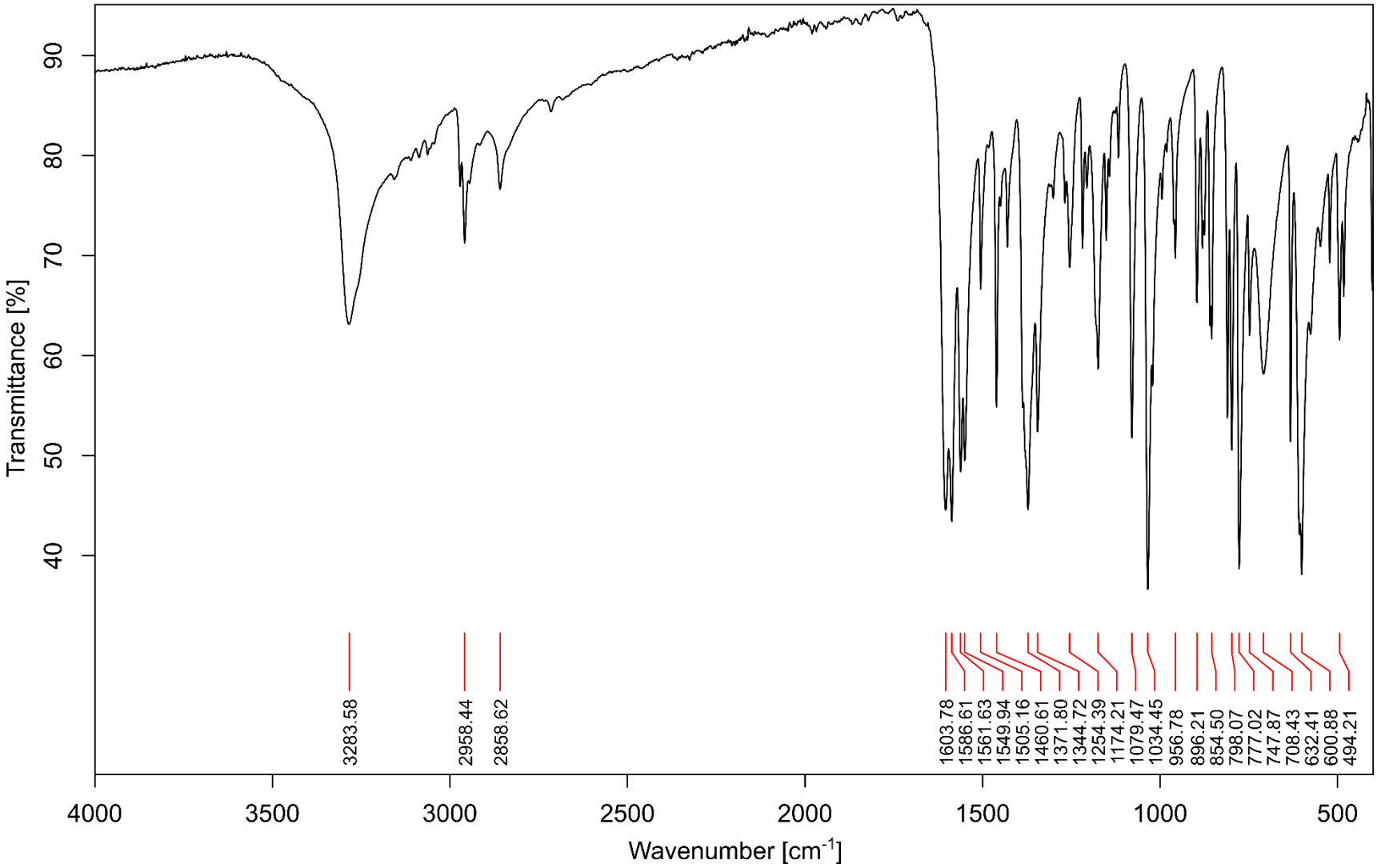


Figure S22. Infrared spectrum of [Cu(quin)$_2$(2maeOH)] (**2b**).

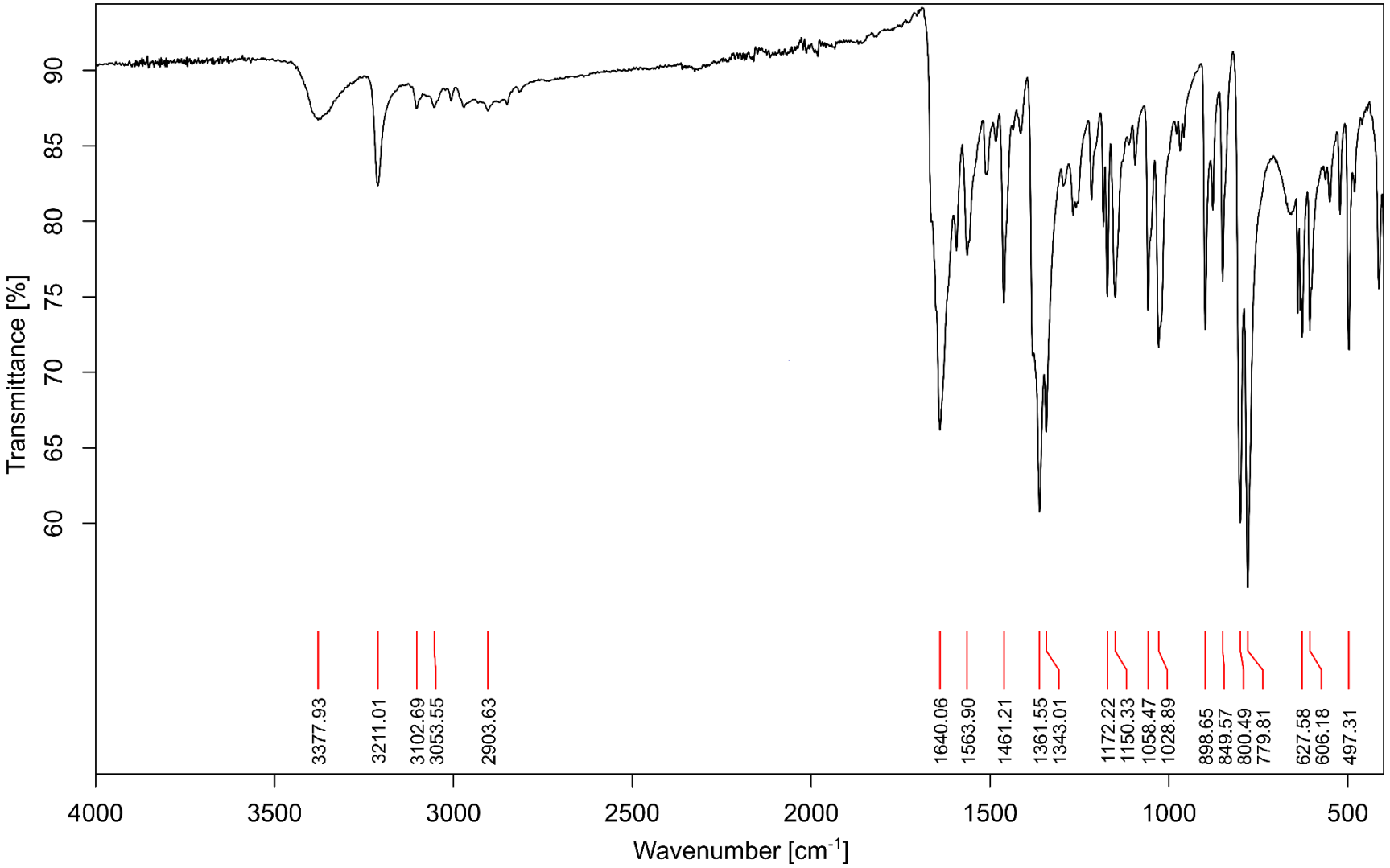


Figure S23. Infrared spectrum of $[Cu(quin)_2]_n$ (**g**).

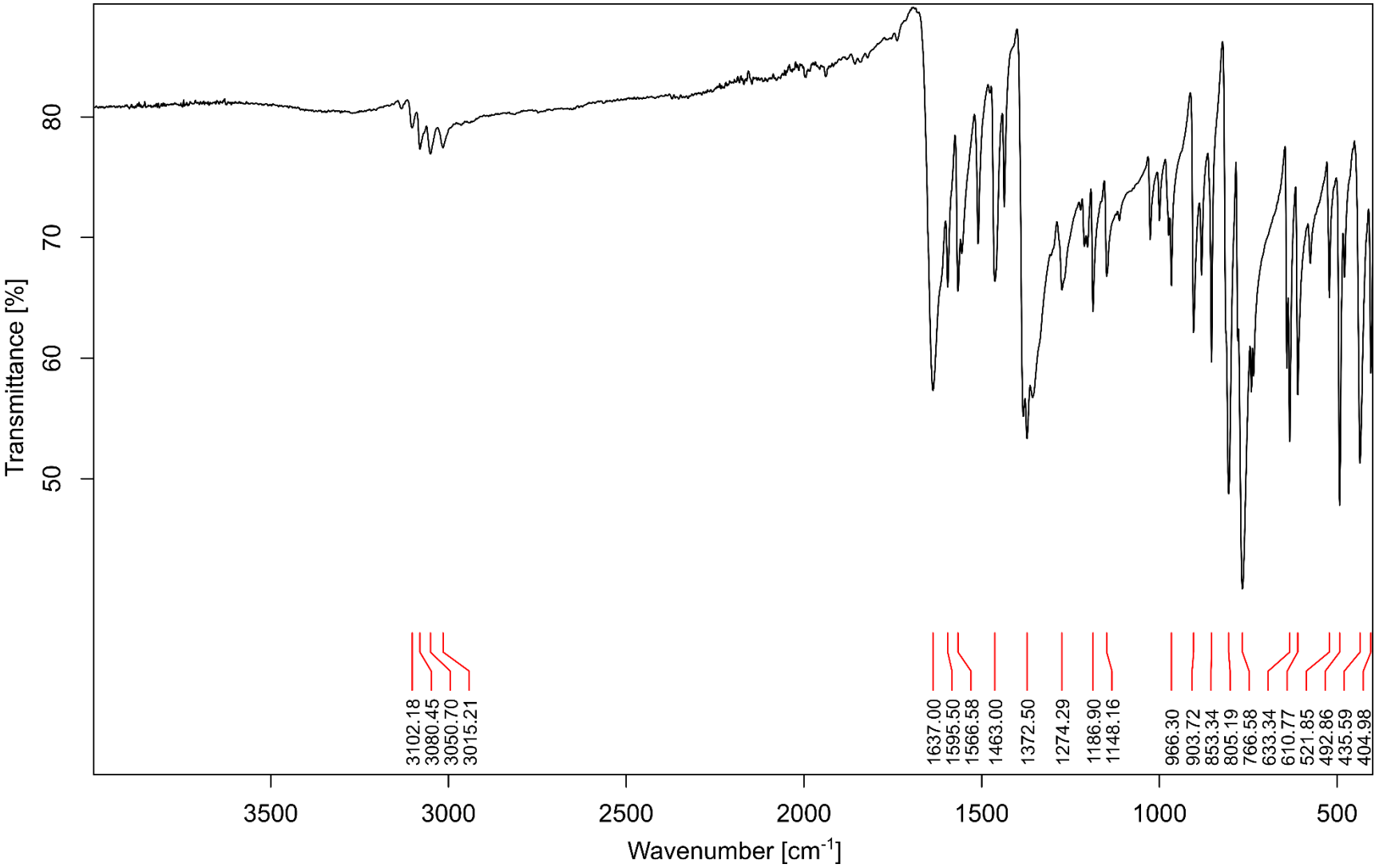


Figure S24. Infrared spectrum of *anti*-[$Cu_2(quin)_2(2eaeO)_2$] (***anti*-4d**).

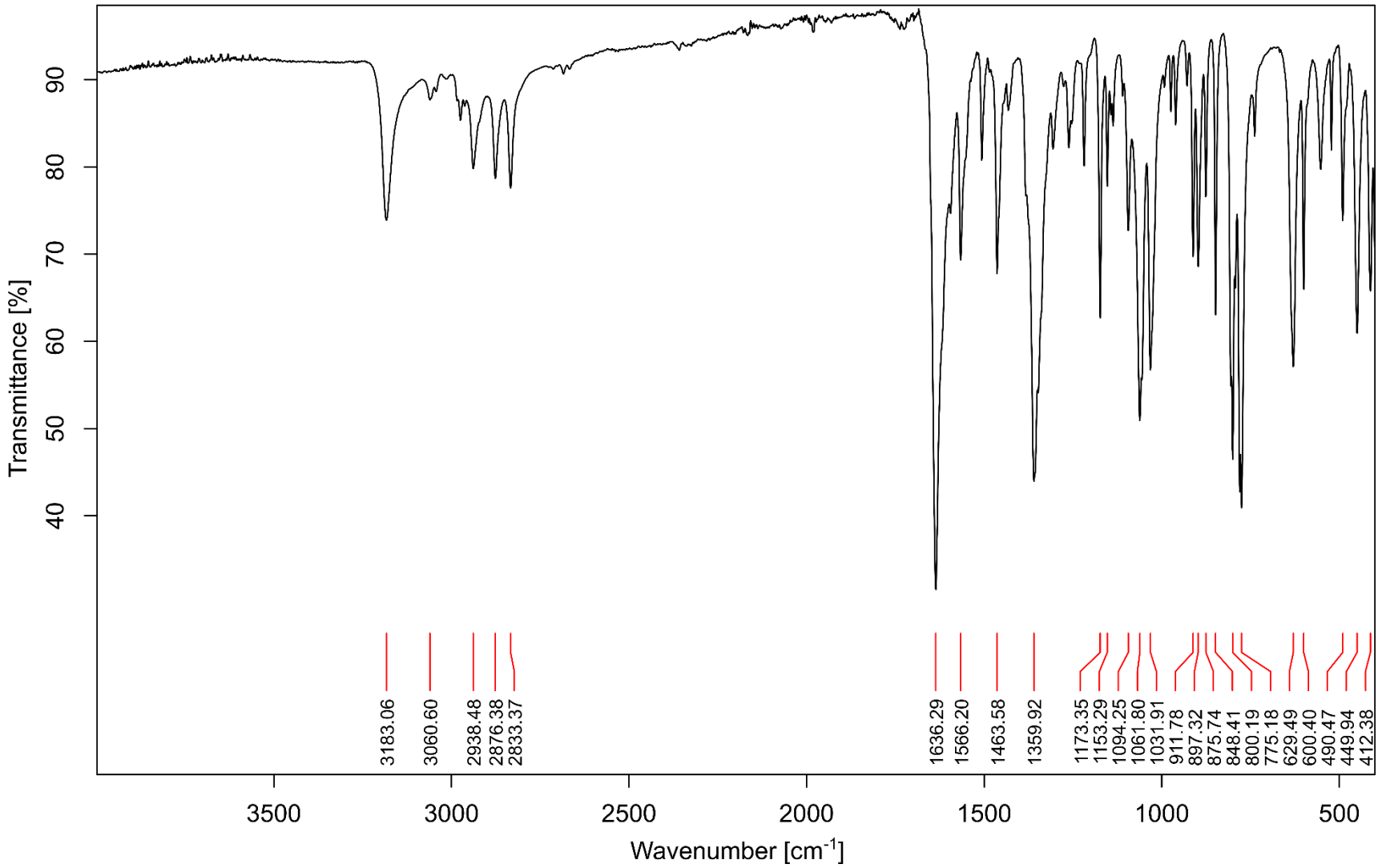


Figure S25. Infrared spectrum of $[Cu(1a2pOH)_3](quin)_2$ (**5e**).

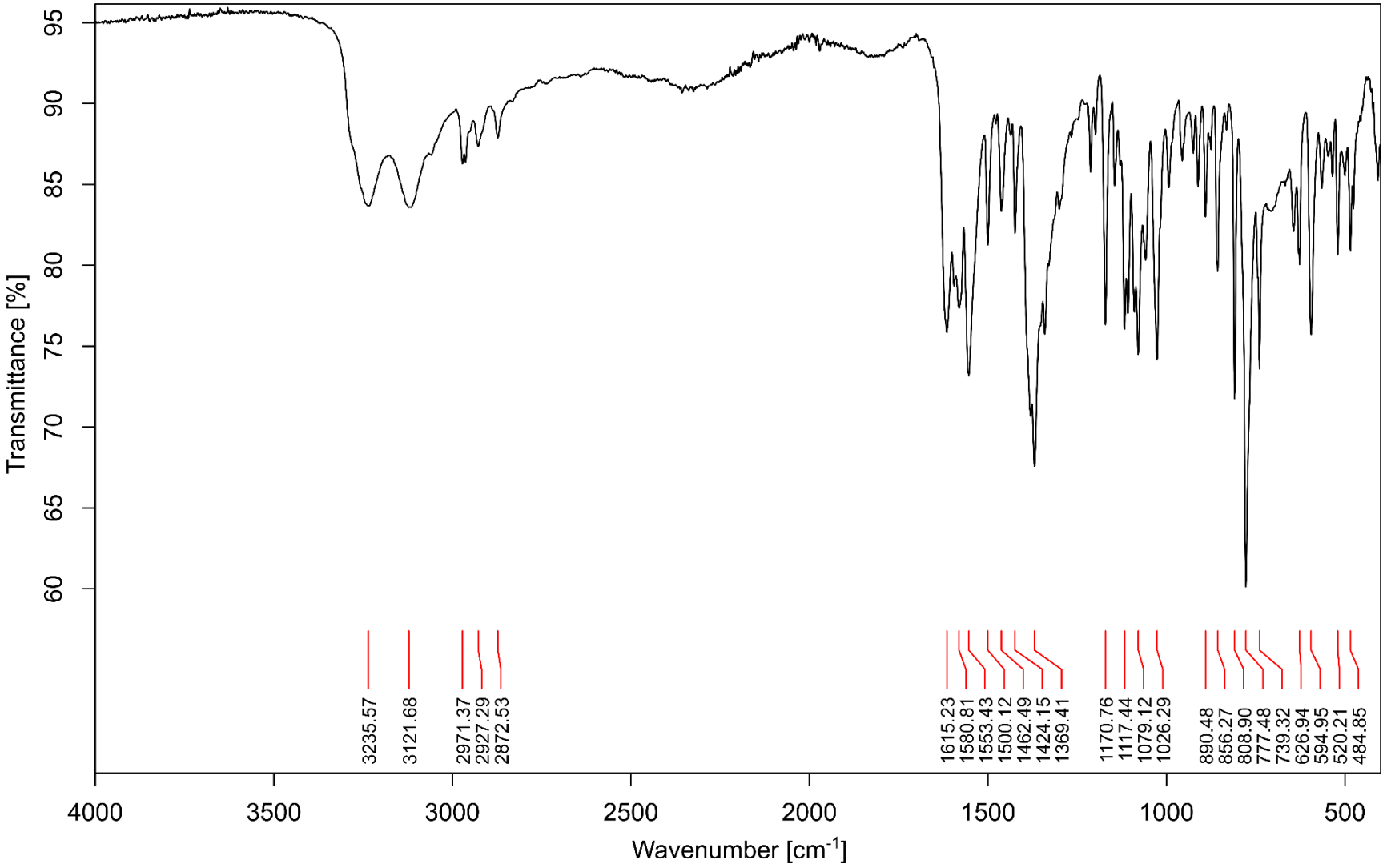


Figure S26. Infrared spectrum of *trans*-[Cu(quin)$_2$(1a2m2pOH)$_2$] (**6a**).

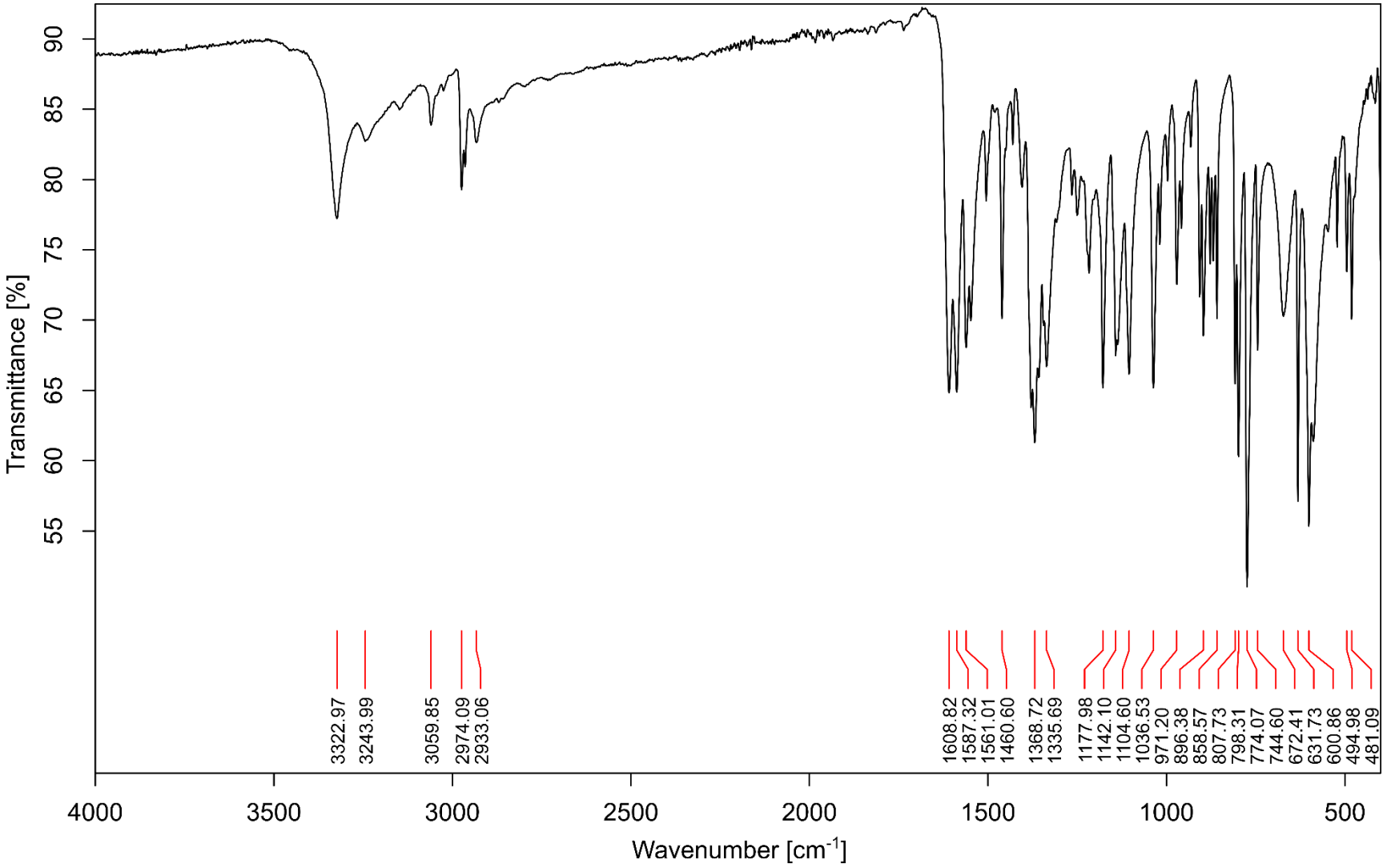


Figure S27. Infrared spectrum of *trans*-[Cu(quin)$_2$(1a2bOH)$_2$] (**7a**).

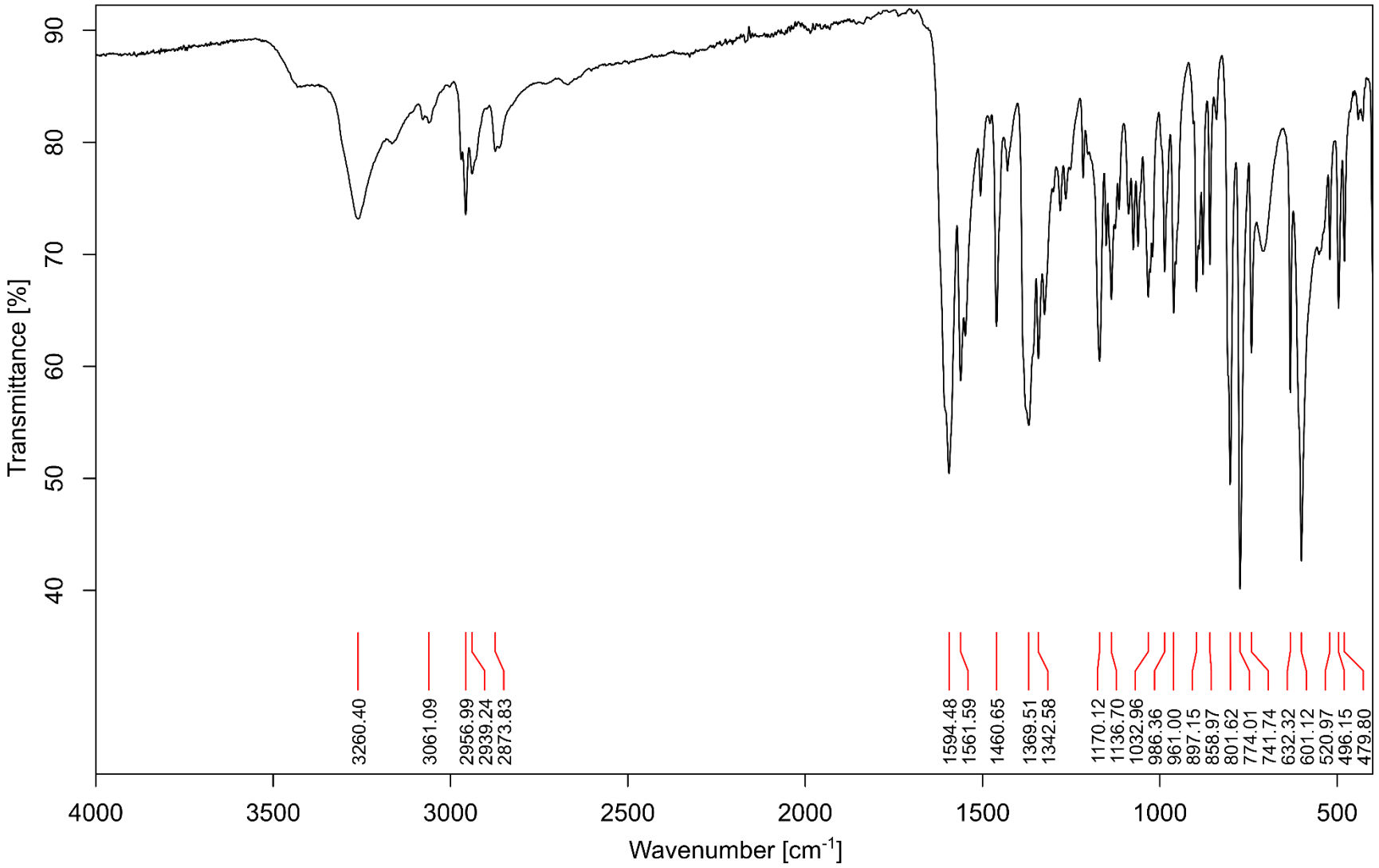


Figure S28. Infrared spectrum of $[Cu(1a2bOH)_3](quin)_2$ (**7e**).

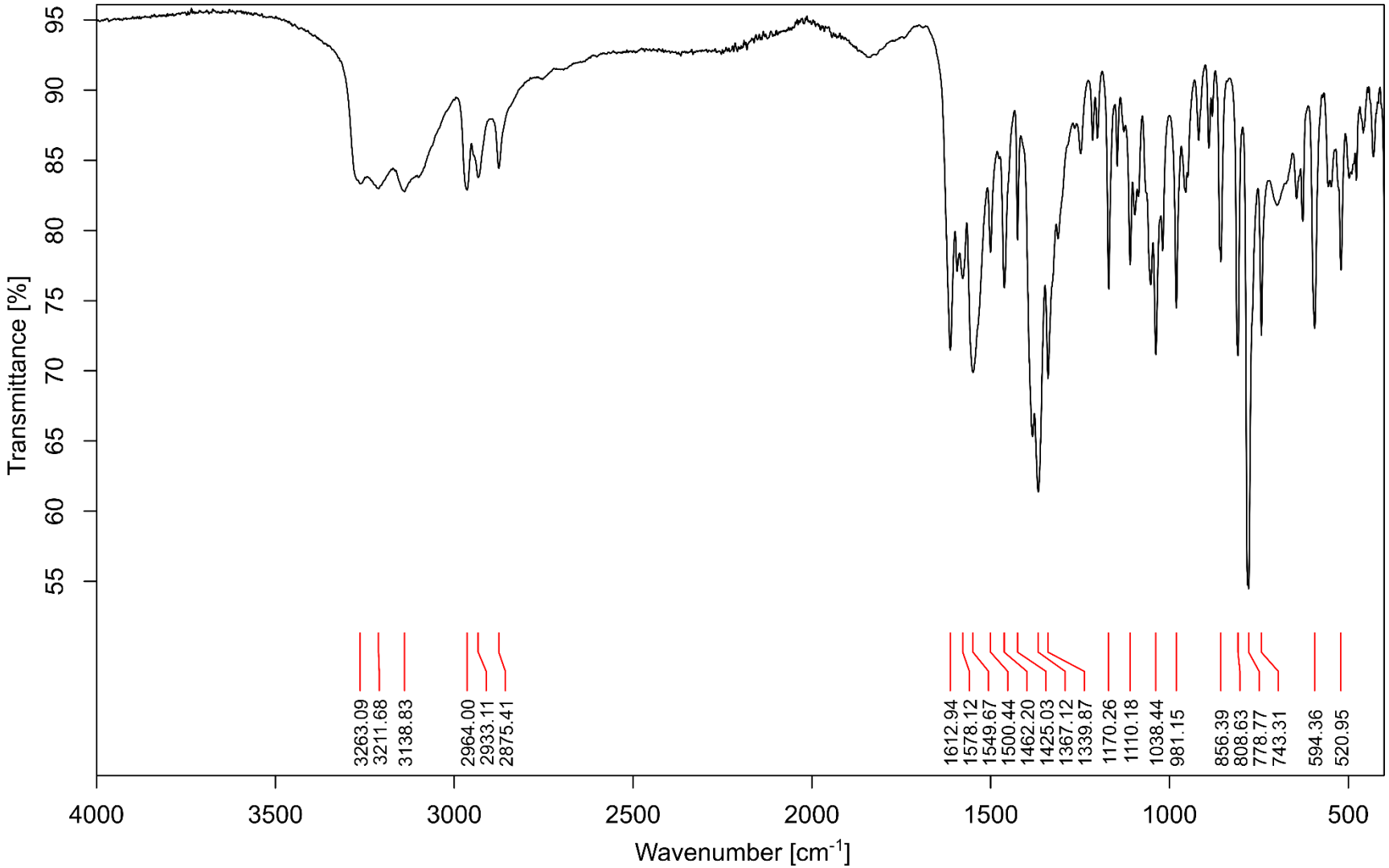


Figure S29. Infrared spectrum of [Cu(quin)$_2$(2a1pOH)] (**8b**).

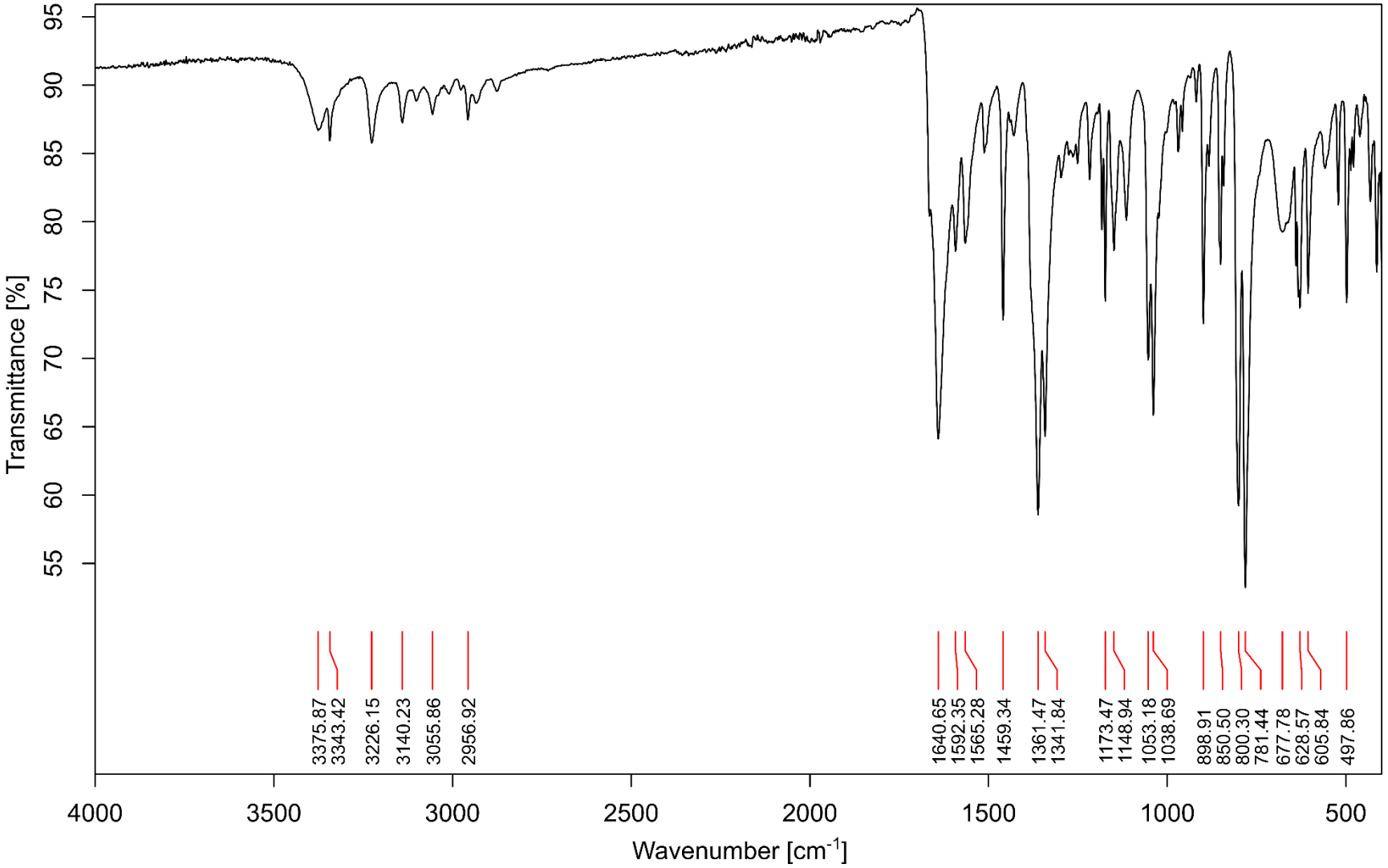


Figure S30. Infrared spectrum of $[Cu(quin)_2(2a1pOH)]_n$ (**8c**).

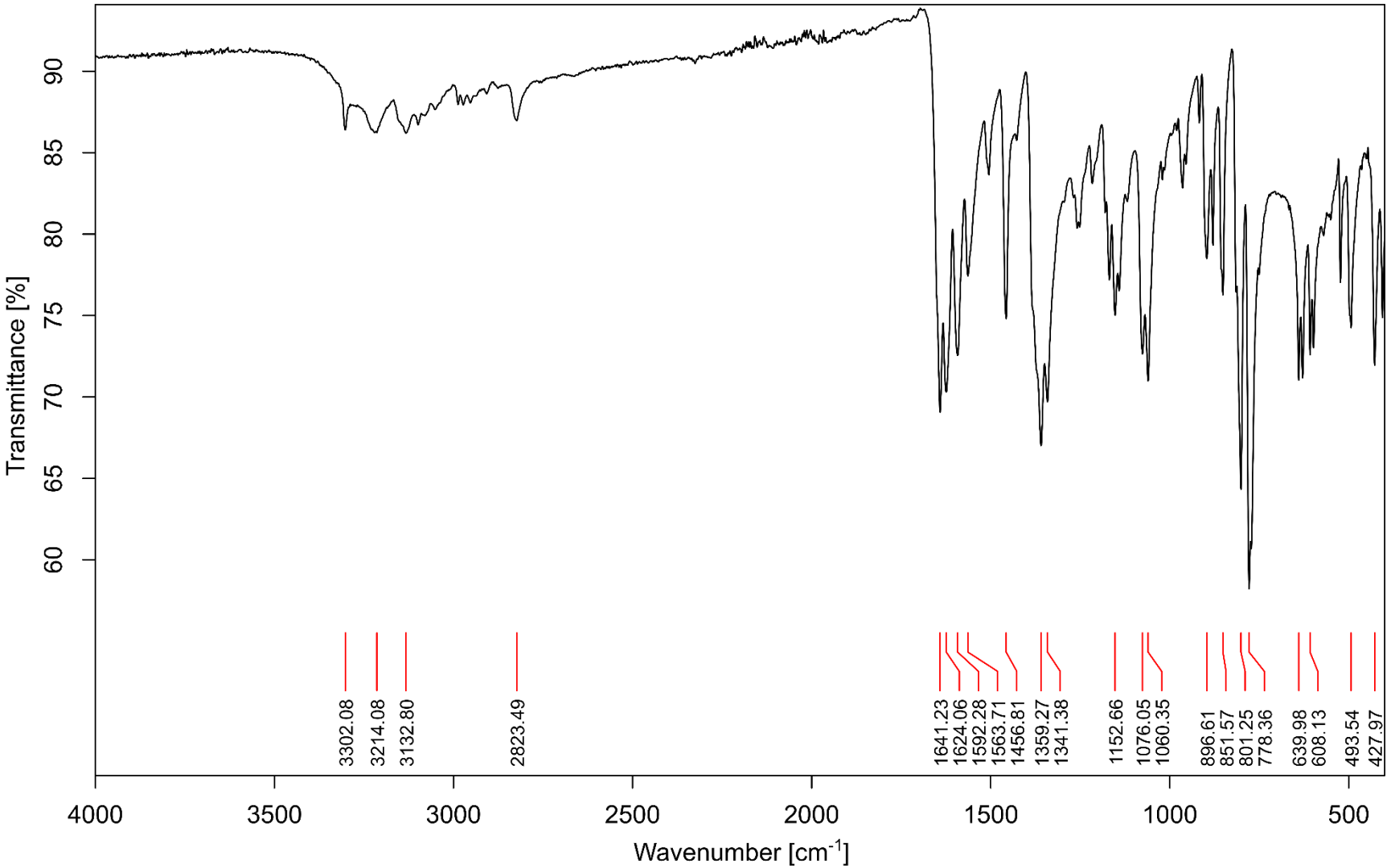


Figure S31. Infrared spectrum of *syn*-[$Cu_2(quin)_2(2a1pO)_2$] (***syn*-8d**).

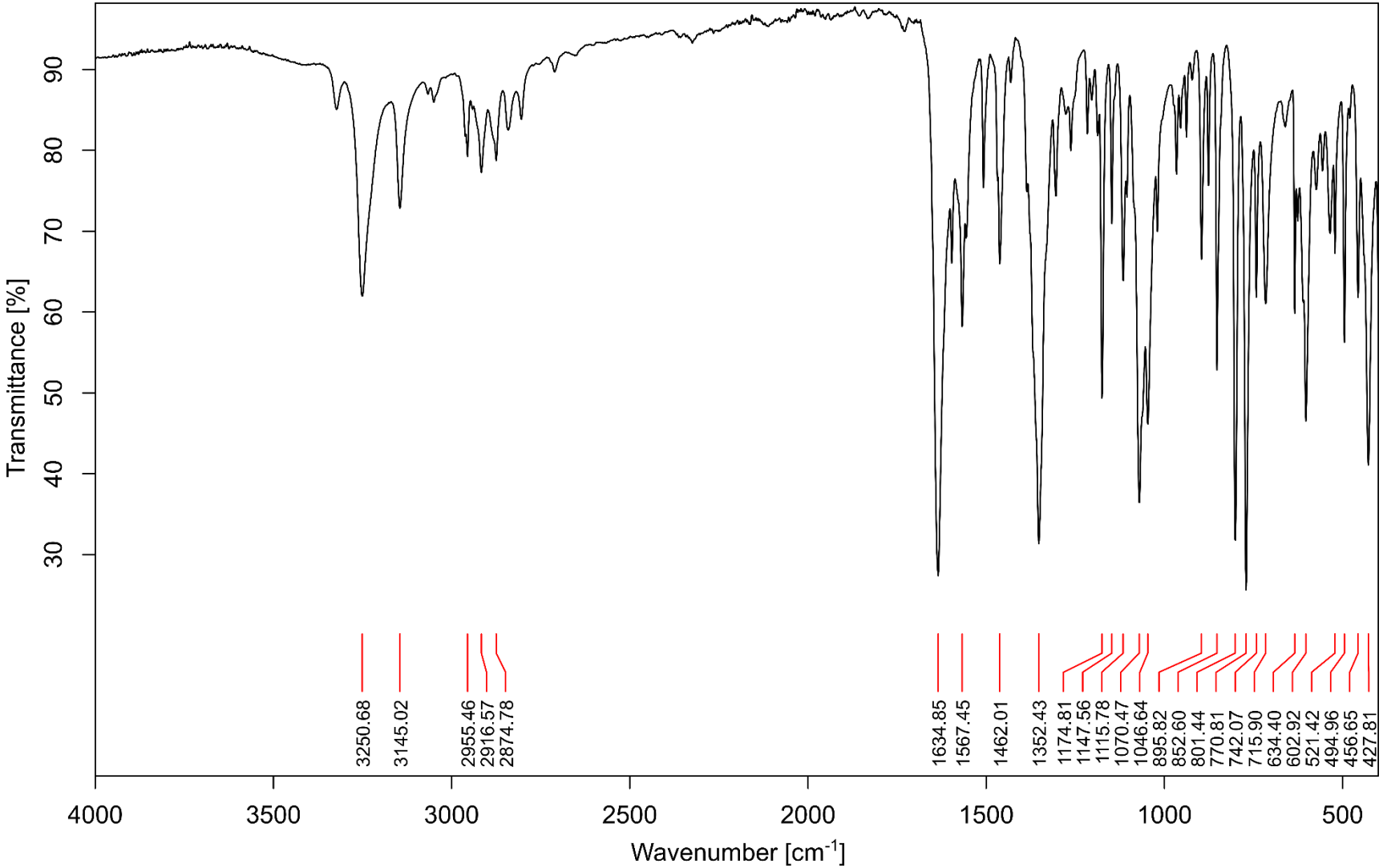


Figure S32. Infrared spectrum of $[Cu(2a1pOH)_3](quin)_2$ (**8e**).

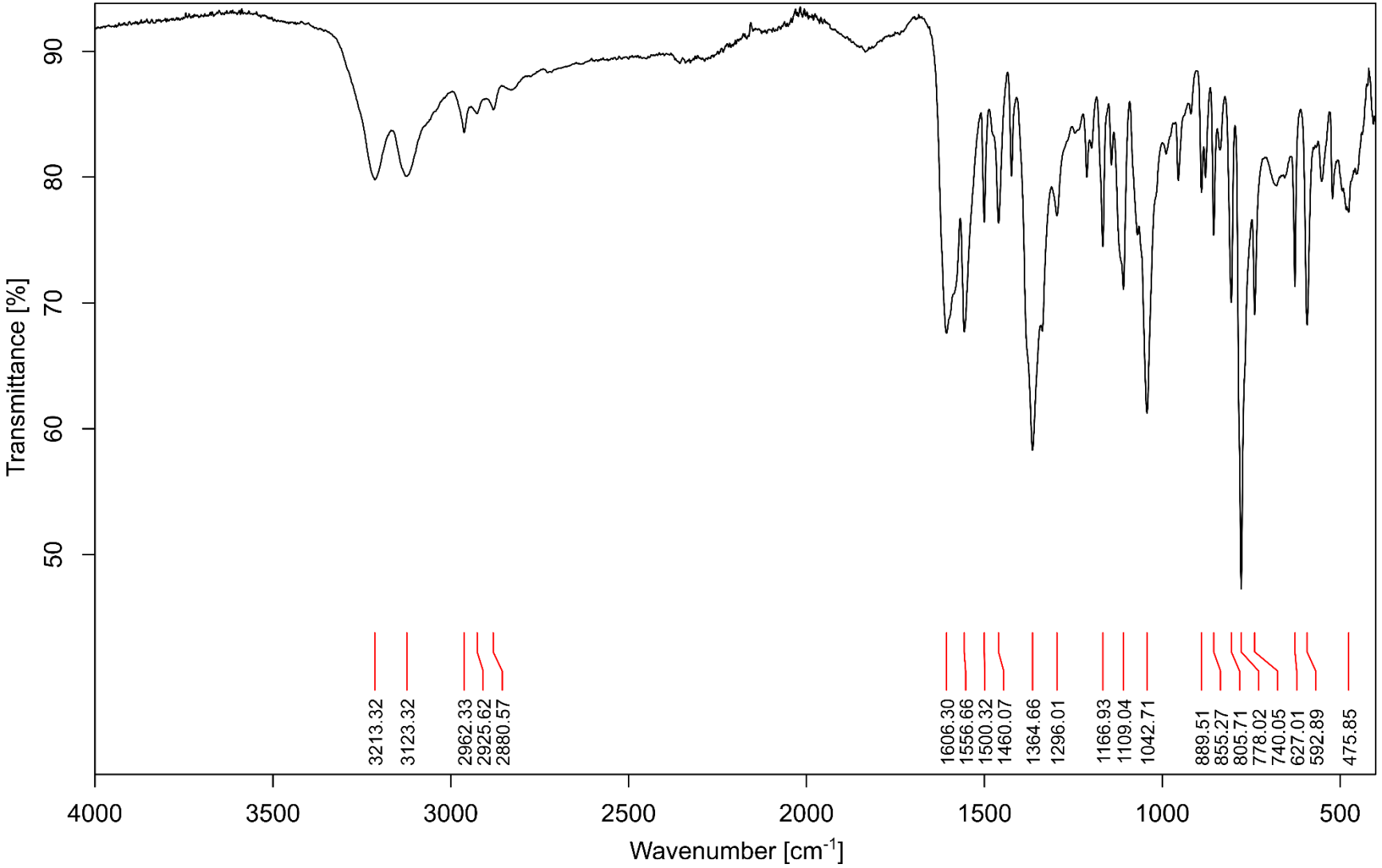


Figure S33. Infrared spectrum of *syn*-[Cu_2(quin)$_2$(2a2m1pO)$_2$] (***syn*-9d**).

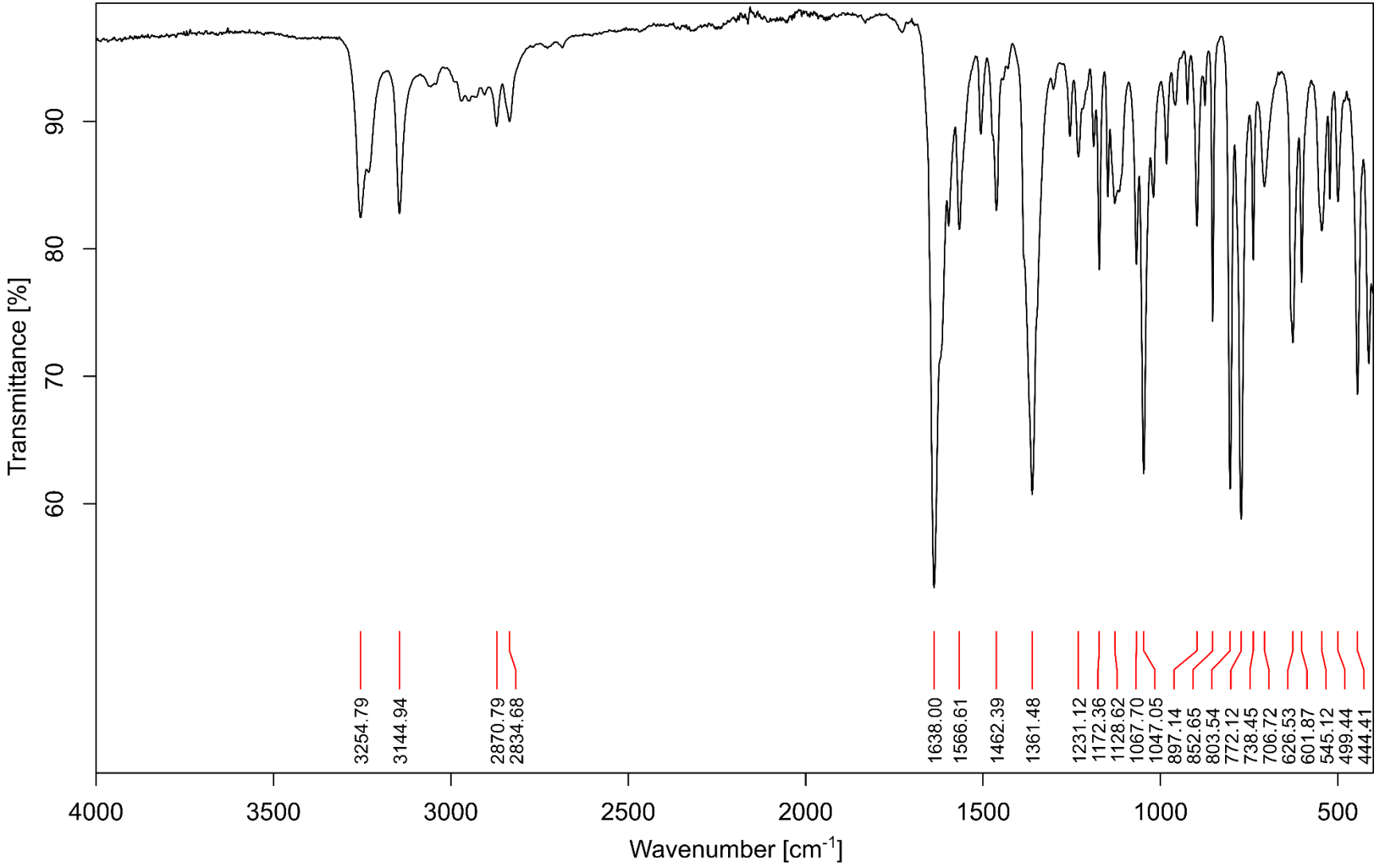


Figure S34. Infrared spectrum of $[Cu(2a2m1pO)_2](2a2m1pOHH)_2(quin)_2$ (**9f**).

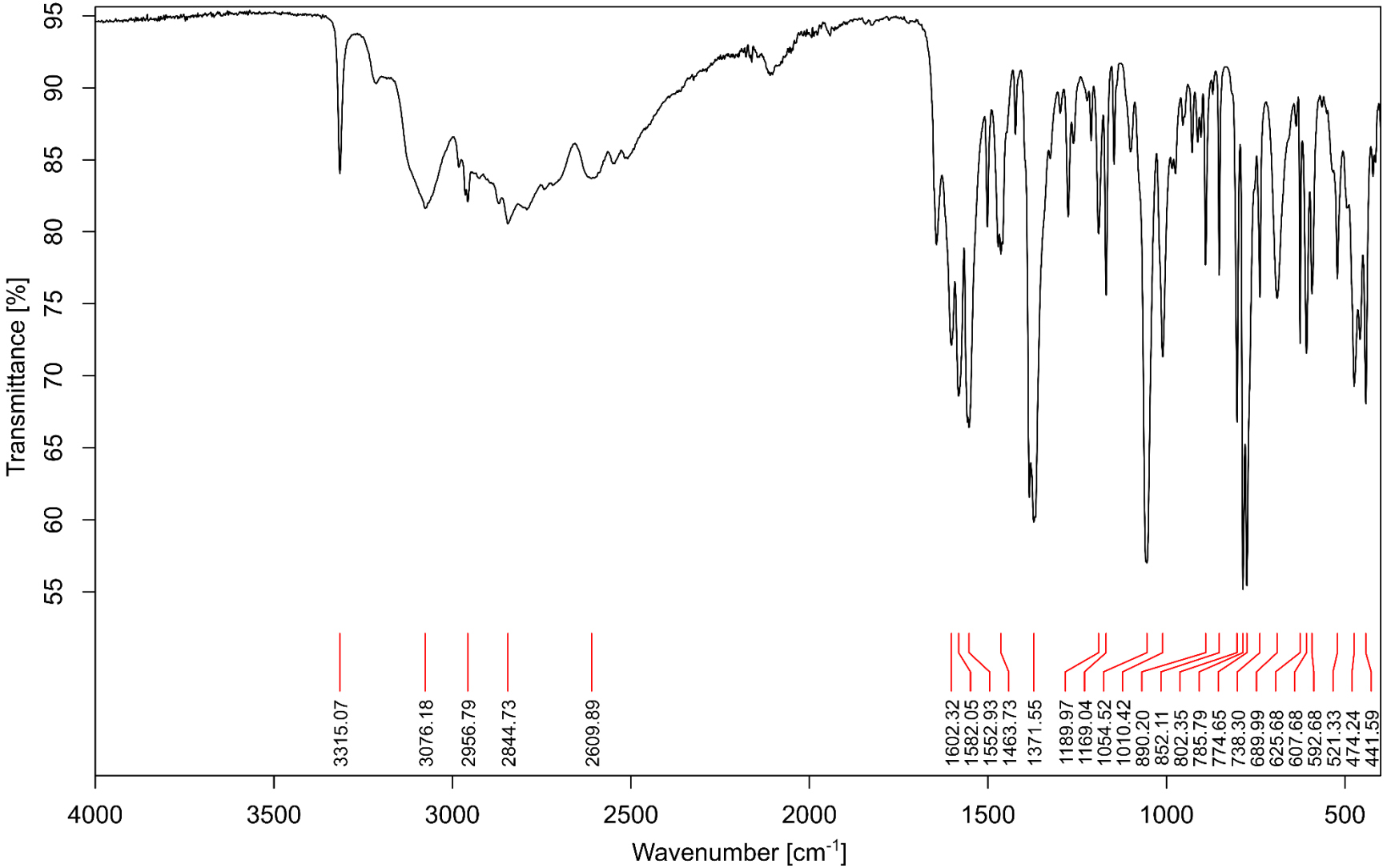


Figure S35. Infrared spectrum of *syn*-[$Cu_2(quin)_2(2a1bO)_2$] (***syn*-10d**).

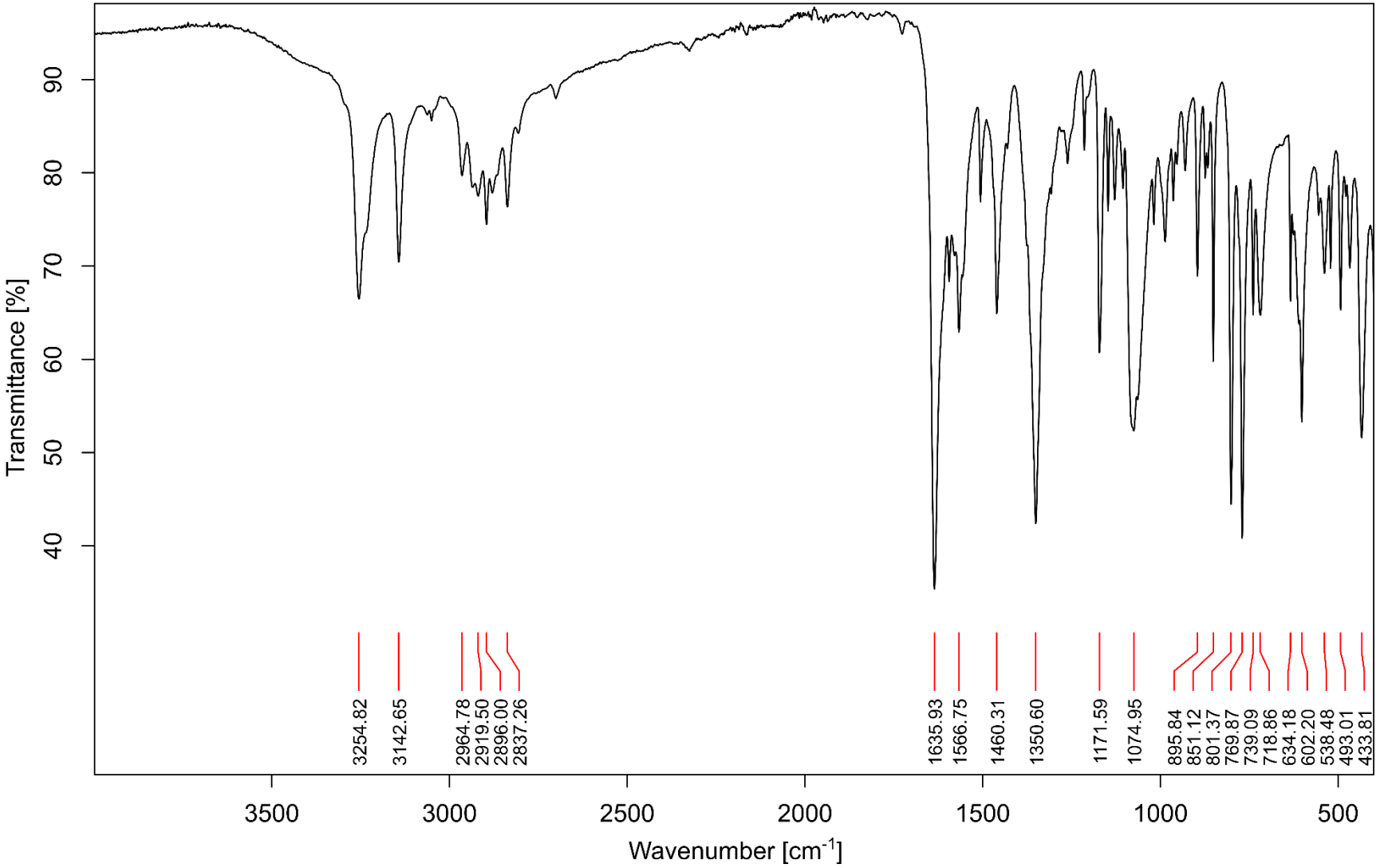


Figure S36. Infrared spectrum of $[Cu(2a1bOH)_3](quin)_2$ (**10e**).

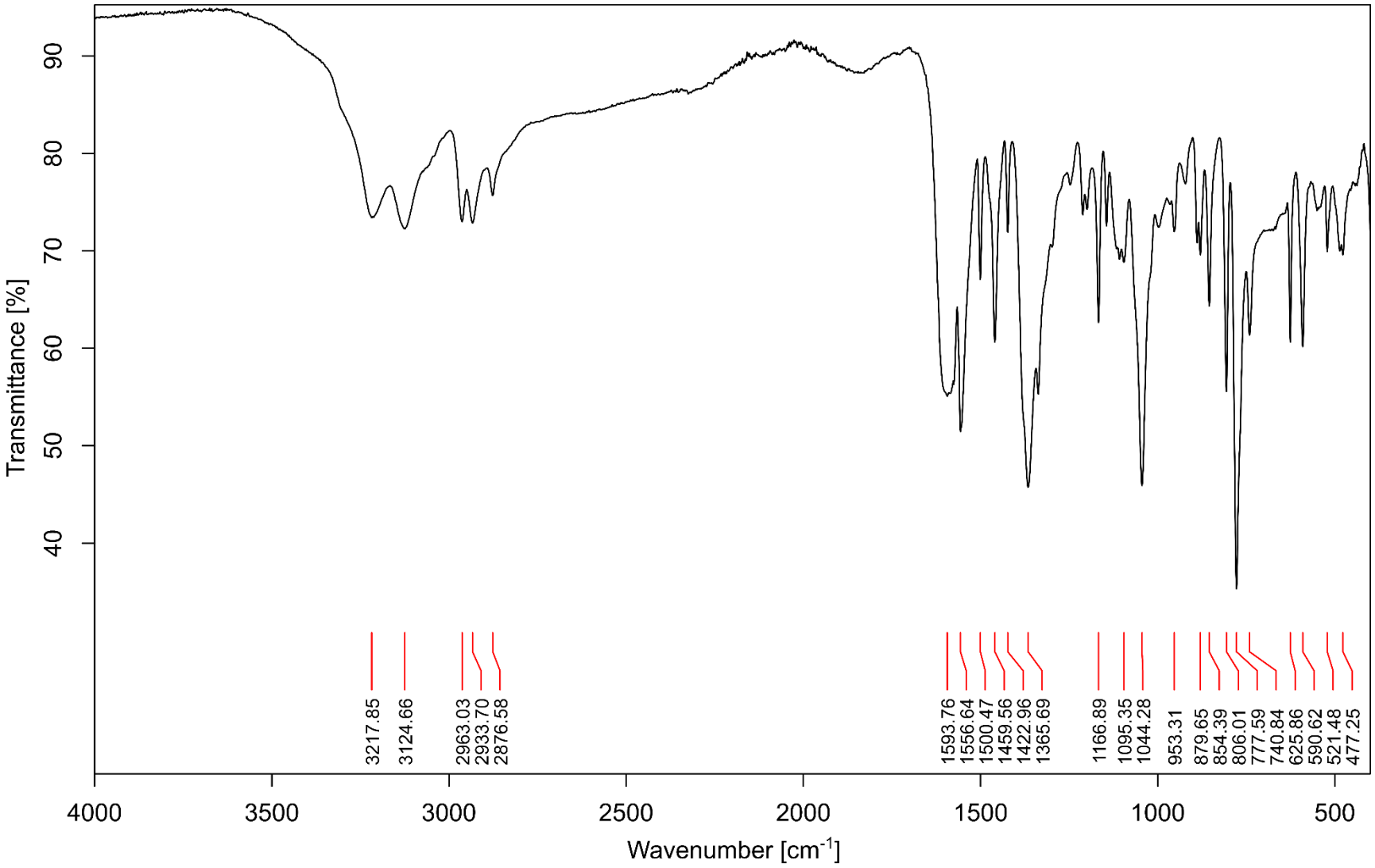


Figure S37. Infrared spectrum of *trans*-[Cu(quin)$_2$(3a1pOH)$_2$] (**11a**).

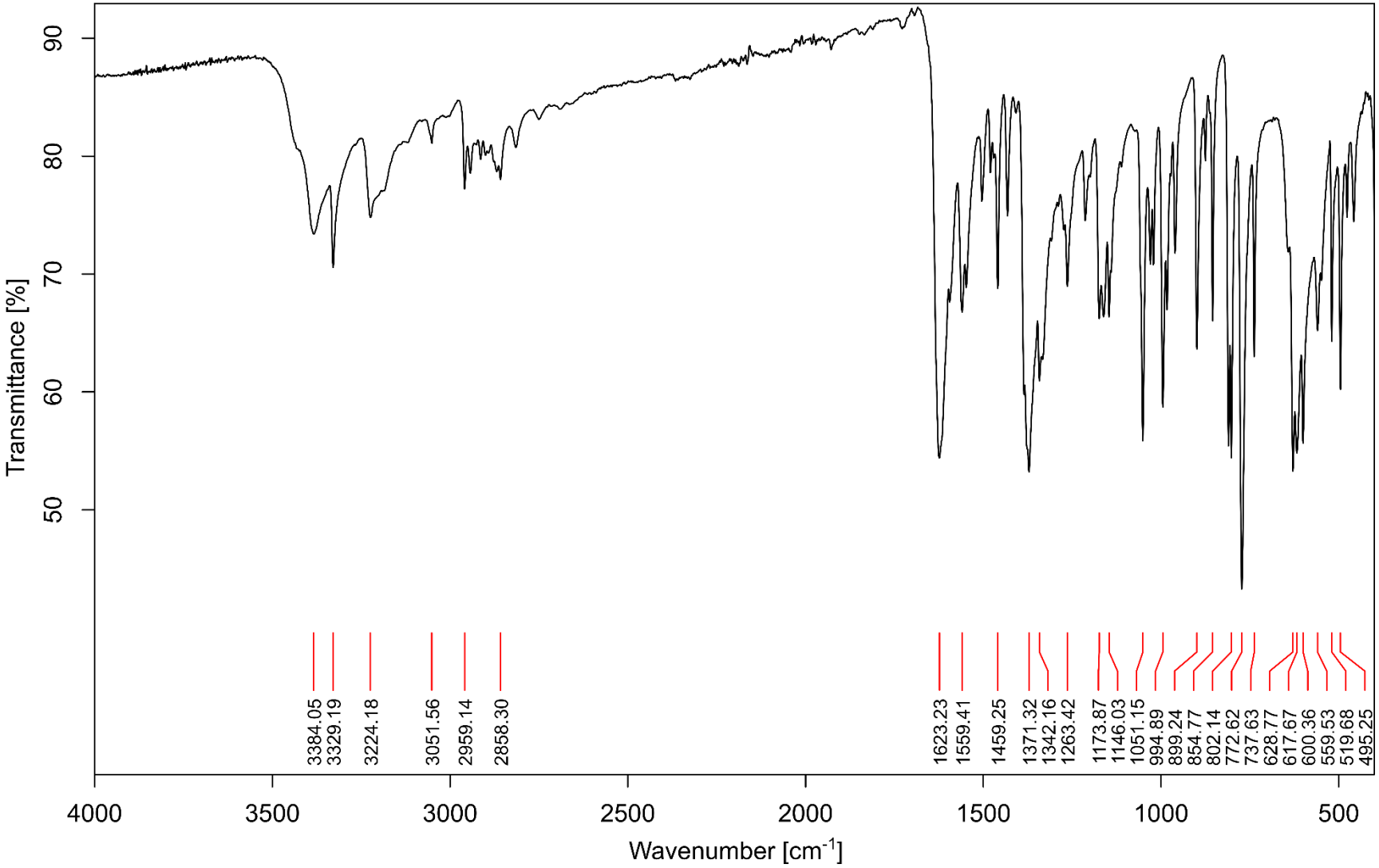


Figure S38. Infrared spectrum of *trans*-[Cu(quin)$_2$(3a1pOH)$_2$]·3a1pOH (**11a·3a1pOH**).

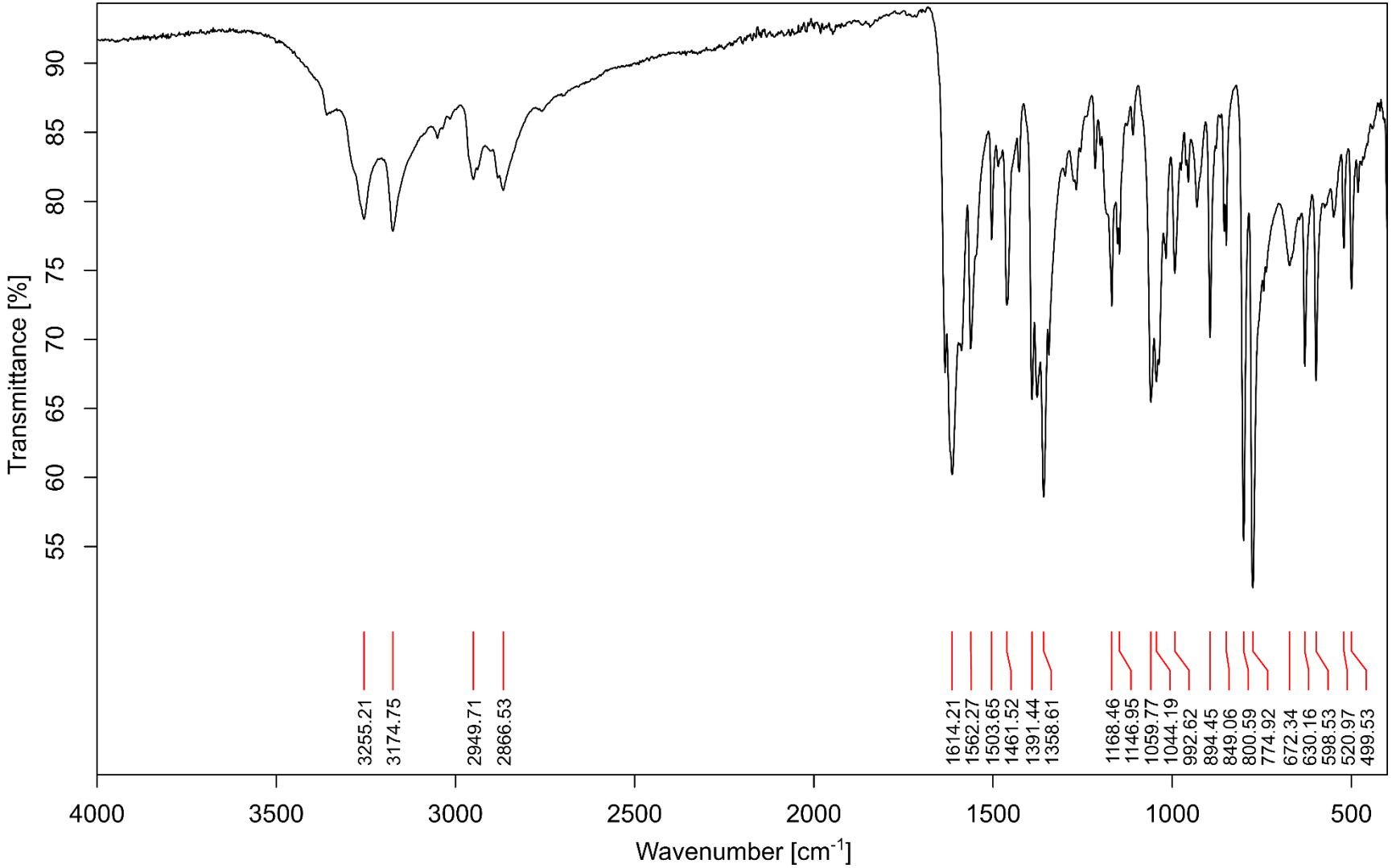


Figure S39. Infrared spectrum of [Cu(quin)$_2$(3a1pOH)] (**11b**).

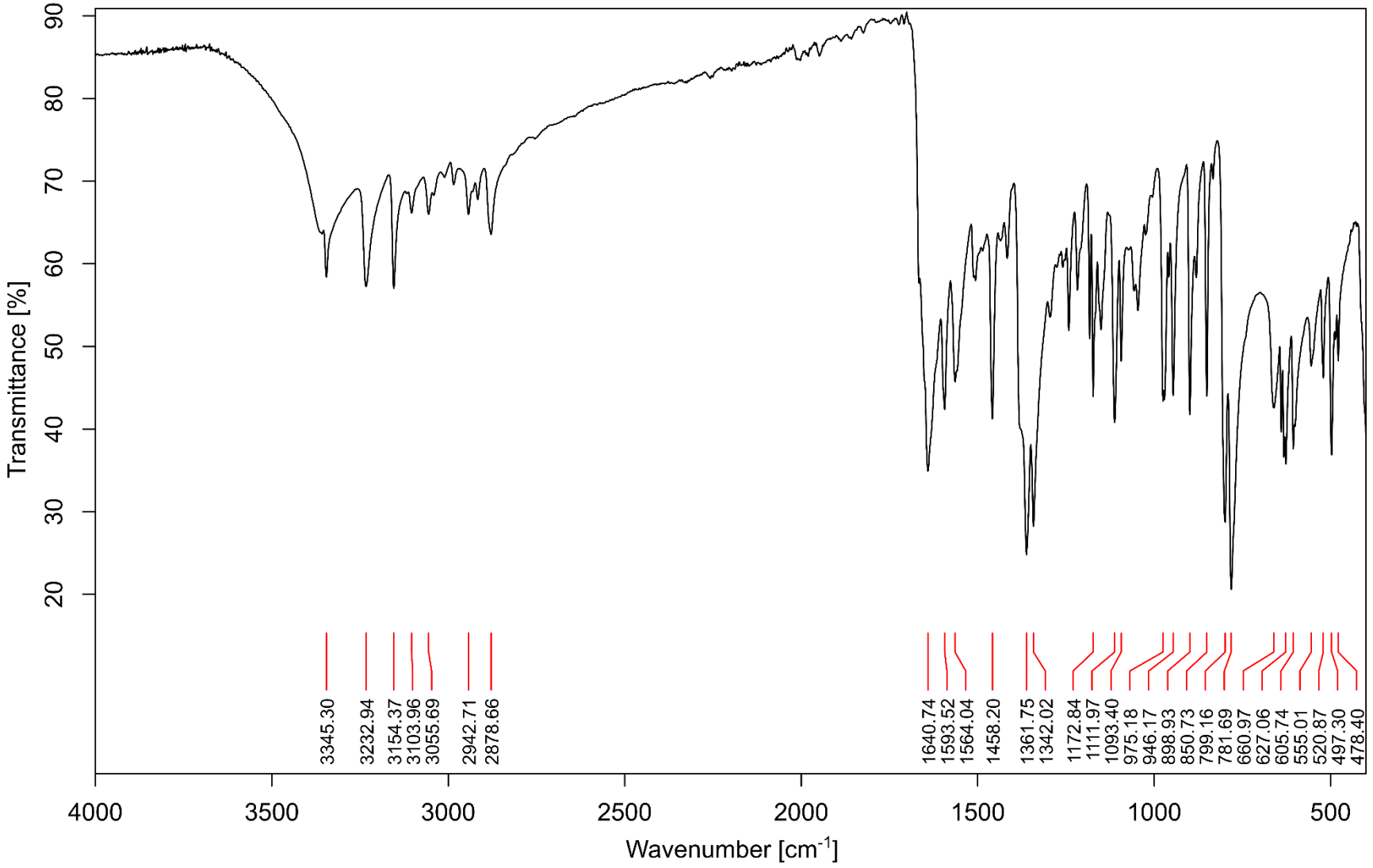


Figure S40. Infrared spectrum of $[Cu(quin)_2(3a1pOH)]_n$ (**11c**).

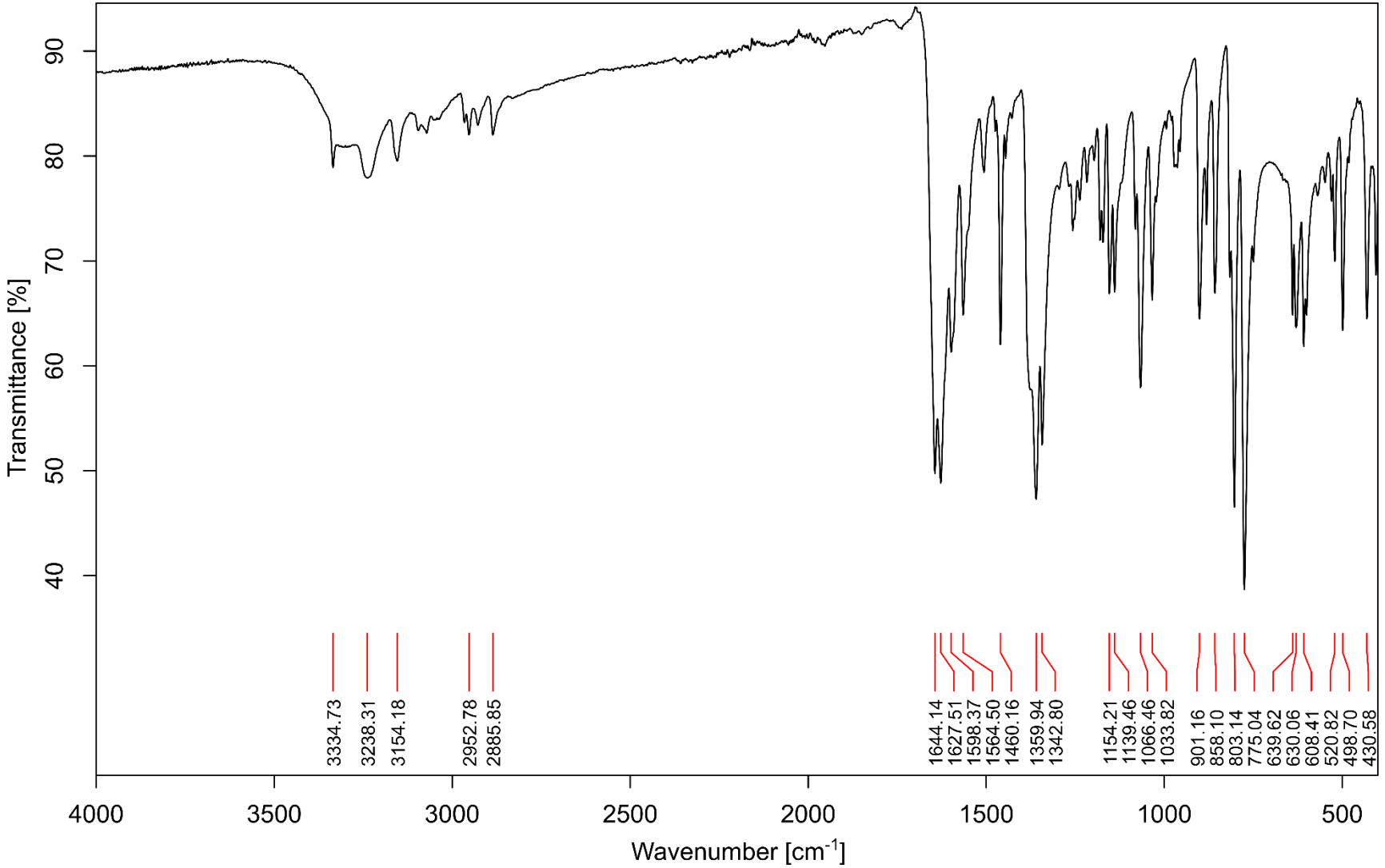


Figure S41. Infrared spectrum of *syn*-$[Cu_2(quin)_2(3a1pO)_2]\cdot 2H_2O$ (***syn*-11d·2H₂O**).

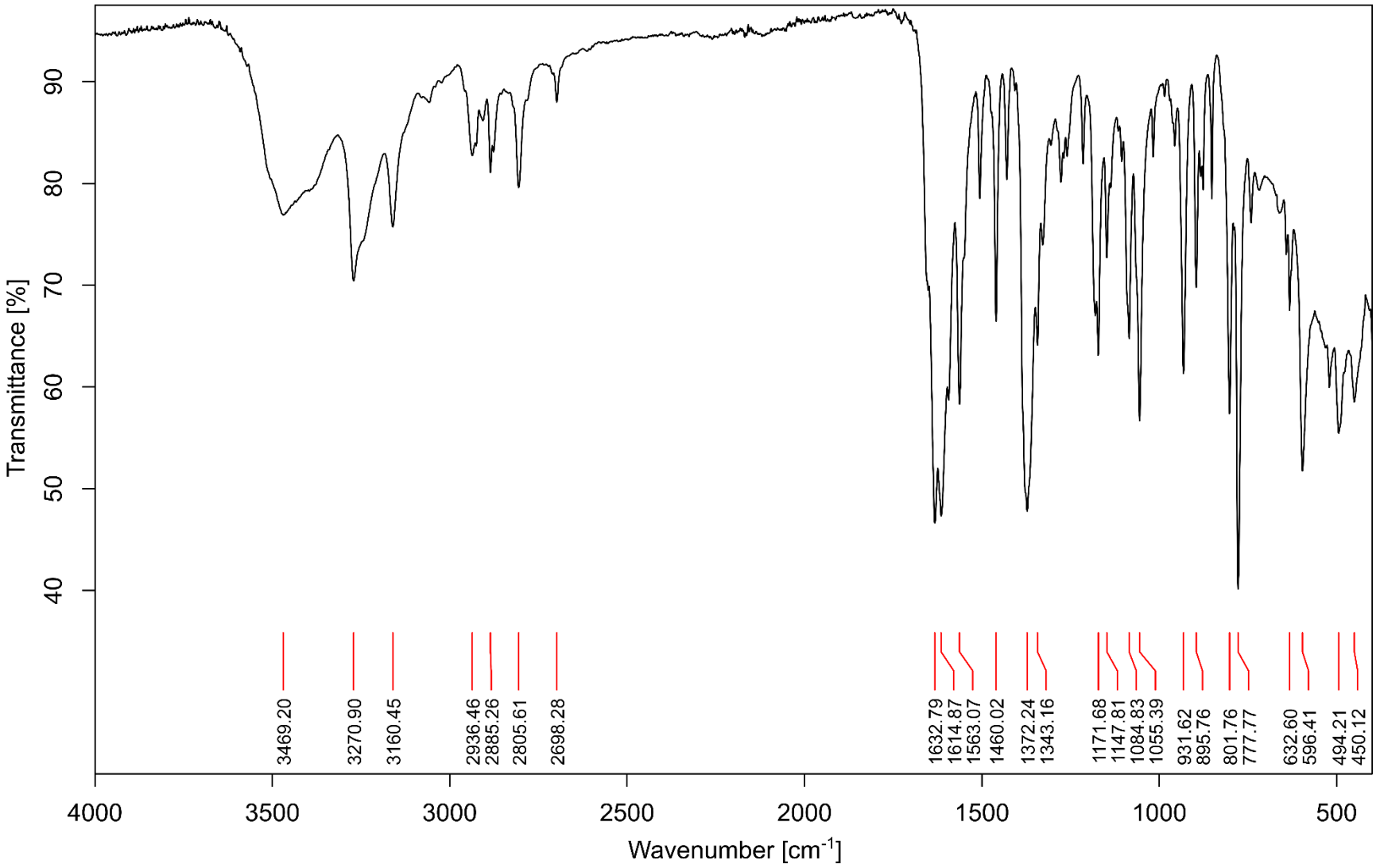


Figure S42. Infrared spectrum of *anti*-[Cu_2(quin)$_2$(3a1pO)$_2$]·2MeCN (***anti*-11d·2MeCN**).

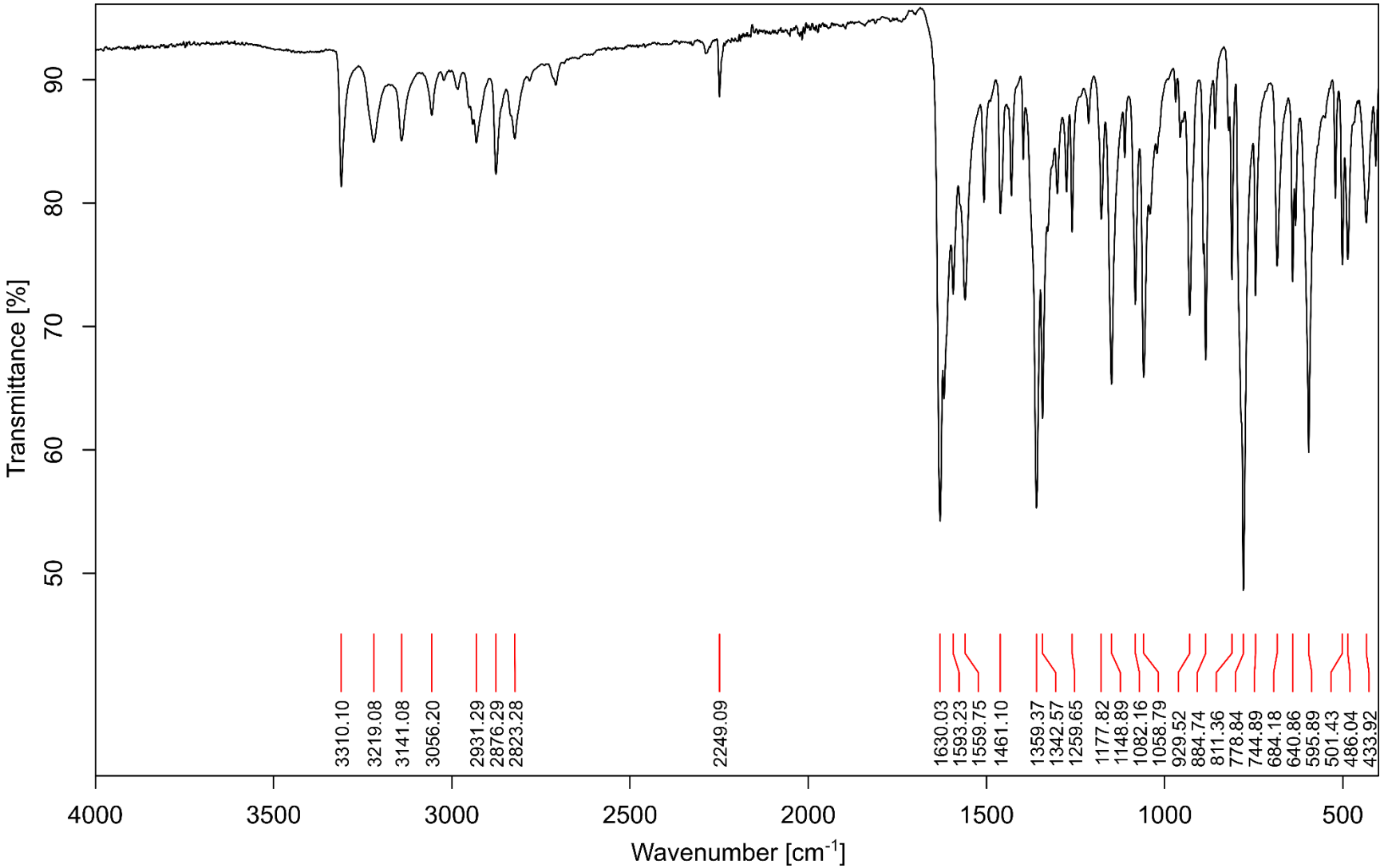


Figure S43. Infrared spectrum of *anti*-[$Cu_2(quin)_2(3a1pO)_2$]·4MeOH (***anti*-11d·4MeOH**).

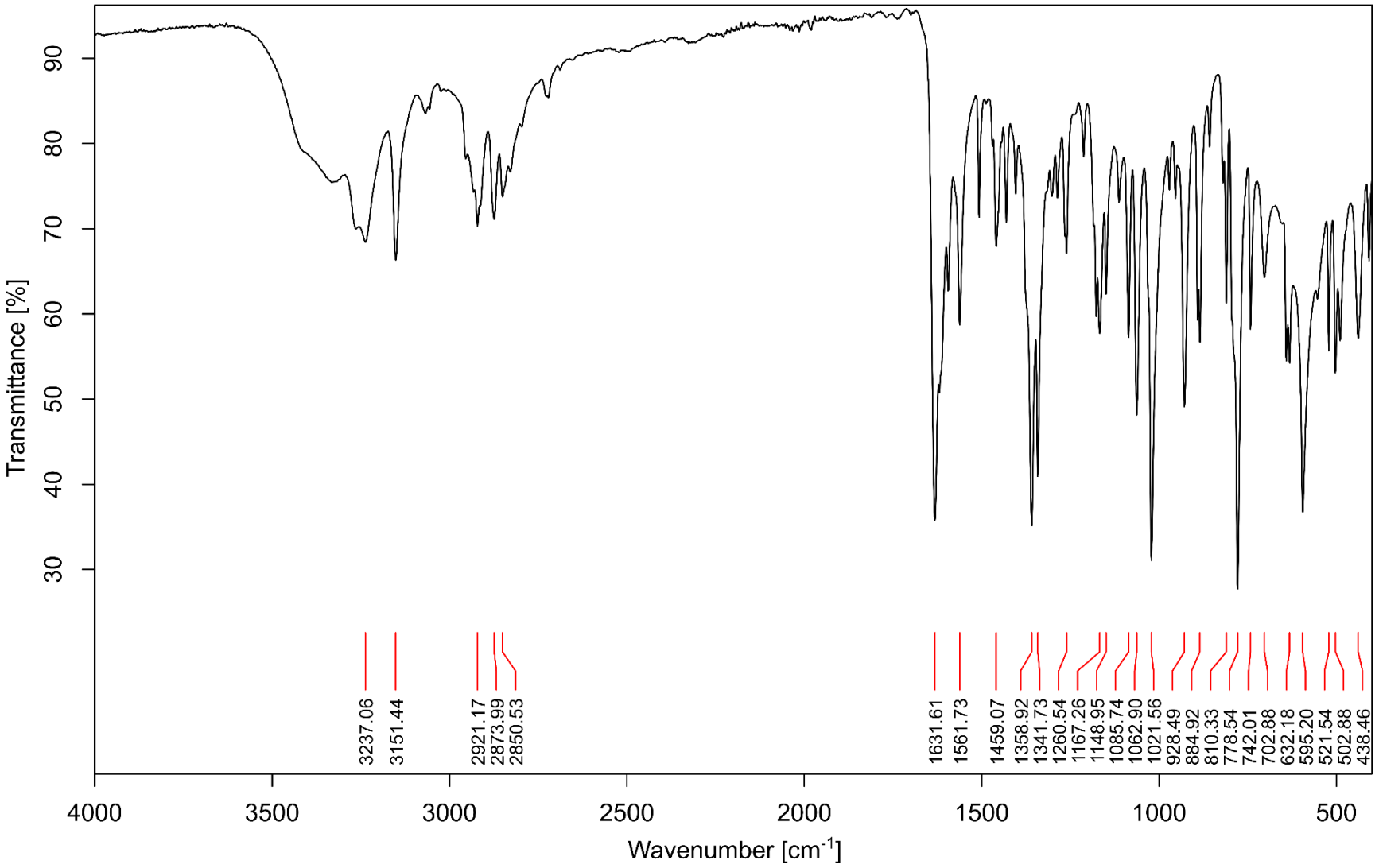


Figure S44. Infrared spectrum of *anti*-[Cu_2(quin)$_2$(3a1pO)$_2$]·2MeOH·2(3a1pOH) (***anti*-11d·2MeOH·2(3a1pOH)**).