Supplementary materials: X-ray crystal structure and geometric isomerism of new copper (II) carboxylate complexes with imidazole derivatives

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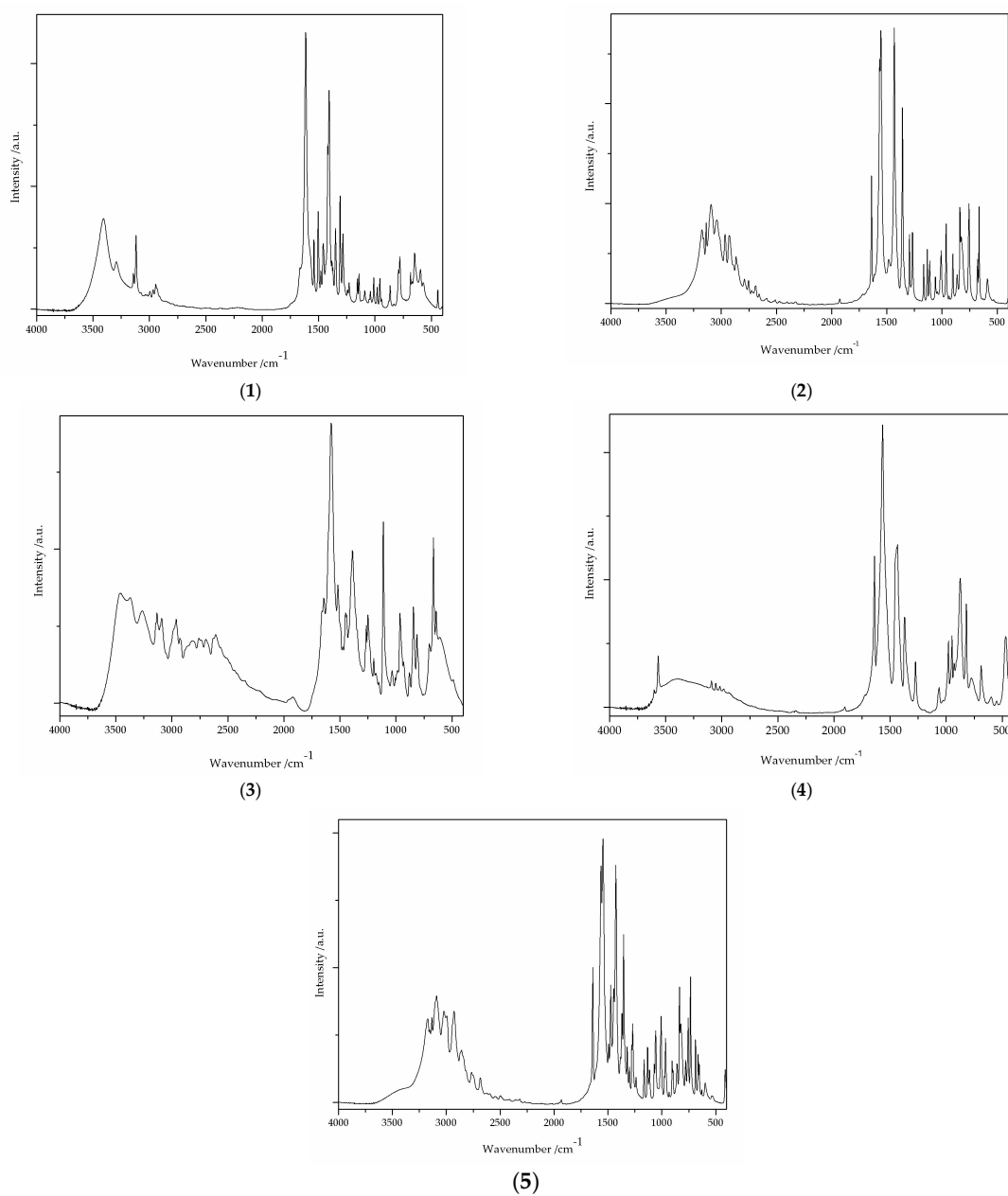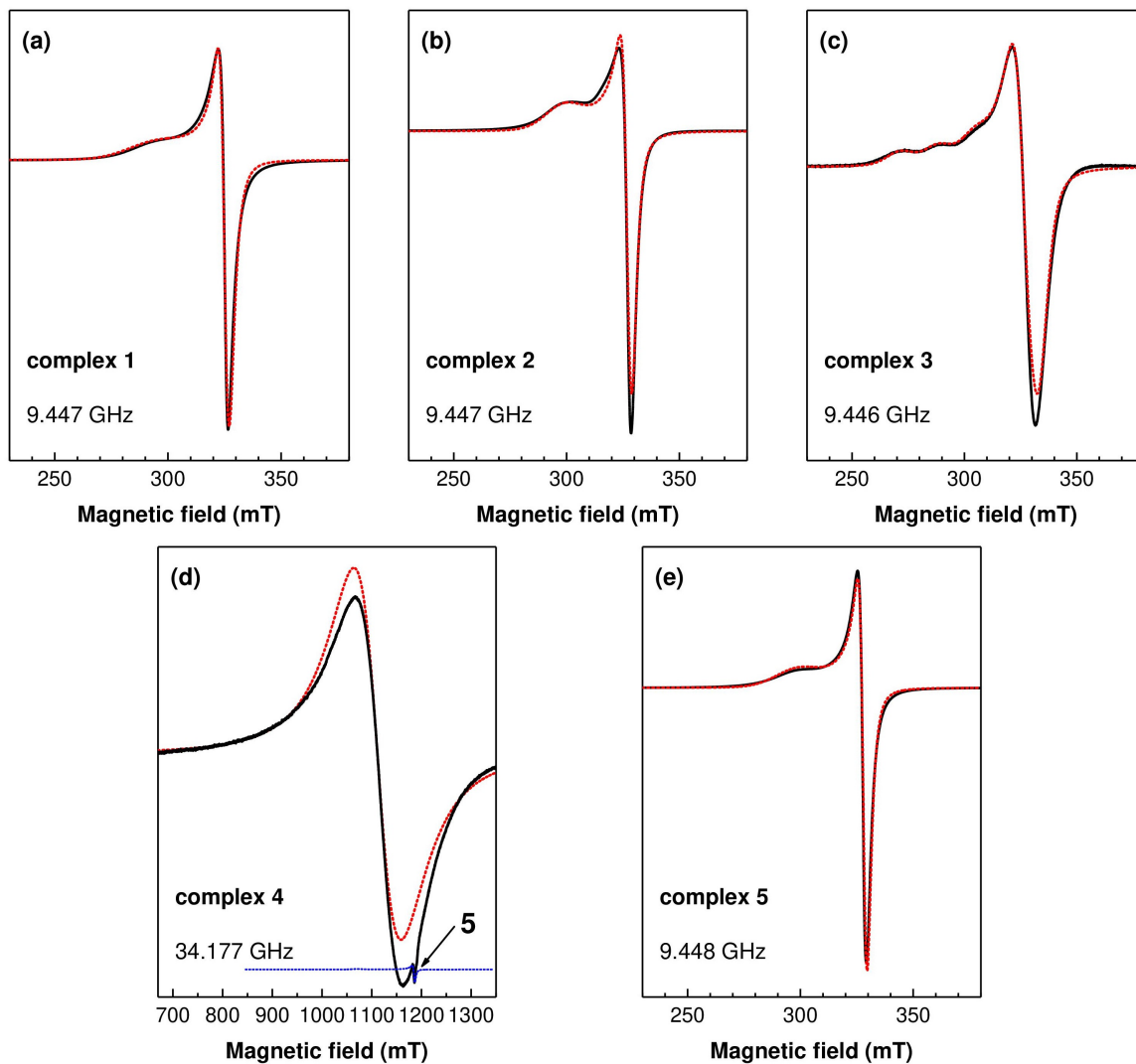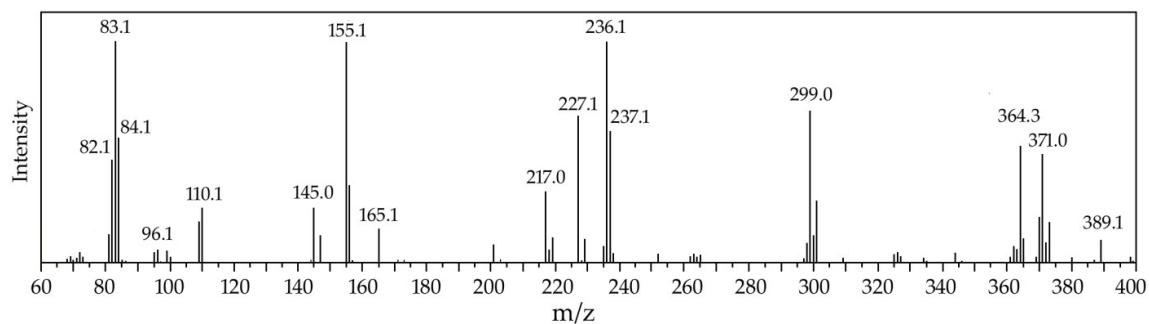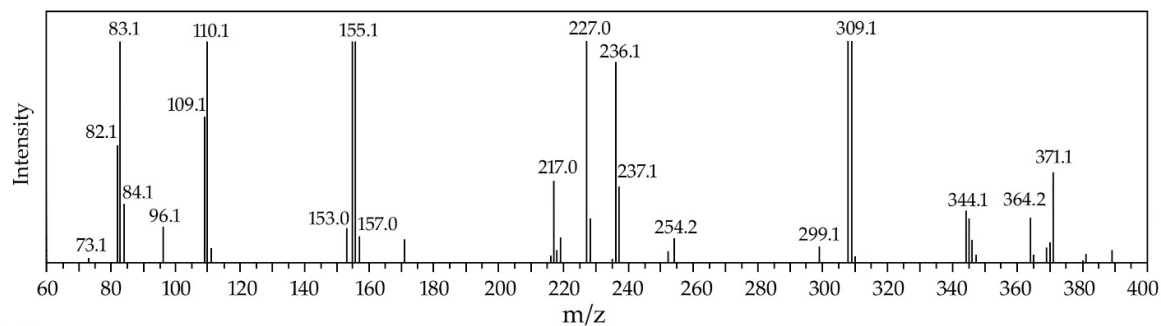
Figure S1. IR spectra of complexes (**1**)-(**5**).

Figure S2. Experimental (solid line) and calculated (dot line) EPR spectra of complexes (**1**)-(**5**).

Table S1. EPR parameters determined for complexes **1-5**.

complex	$g_\parallel$	$g_\perp$	$A_\parallel$ [10^{-4} cm^{-1}]	$A_\perp$ [10^{-4} cm^{-1}]	$G = (g_\parallel - 2)/(g_\perp - 2)$
1	2.322 ± 0.003	2.069 ± 0.003	-	-	4.67
2	2.268 ± 0.003	2.057 ± 0.003	-	-	4.70
3	2.277 ± 0.003	2.060 ± 0.003	173 ± 5	14 ± 5	4.62
4	$g_\parallel = g_\perp = 2.197 \pm 0.005$		-	-	
5	2.273 ± 0.003	2.055 ± 0.003			4.96

Table S2. Absorption maxima in UV-Vis-NIR spectra of complexes (**1**)-(**5**).

Complex	Absorption maxima (nm)	Assignments
[Cu(2-MeIm)$_2$(acr)$_2$]·2H$_2$O (**1**)	260	$\pi \rightarrow \pi^*$
	655	$d_{xz,yz} \rightarrow d_{x^2-y^2}$
[Cu(2-MeIm)$_2$(acr)$_2$] (**2**)	275 320	$\pi \rightarrow \pi^*$
	555	$d_{xz,yz} \rightarrow d_{x^2-y^2}$
	690	$d_{z^2} \rightarrow d_{x^2-y^2}$
[Cu(5-MeIm)$_2$(acr)$_2$] (**3**)	250 315	$\pi \rightarrow \pi^*$
	575	$d_{xz,yz} \rightarrow d_{x^2-y^2}$
	675	$d_{z^2} \rightarrow d_{x^2-y^2}$
[Cu(2-EtIm)$_2$(acr)$_2$] (**4**)	295	$\pi \rightarrow \pi^*$
	665	$d_{xz,yz} \rightarrow d_{x^2-y^2}$
[Cu(2-EtIm)$_2$(acr)$_2$] (**5**)	300	$\pi \rightarrow \pi^*$
	595	$d_{xz,yz} \rightarrow d_{x^2-y^2}$
	690	$d_{z^2} \rightarrow d_{x^2-y^2}$

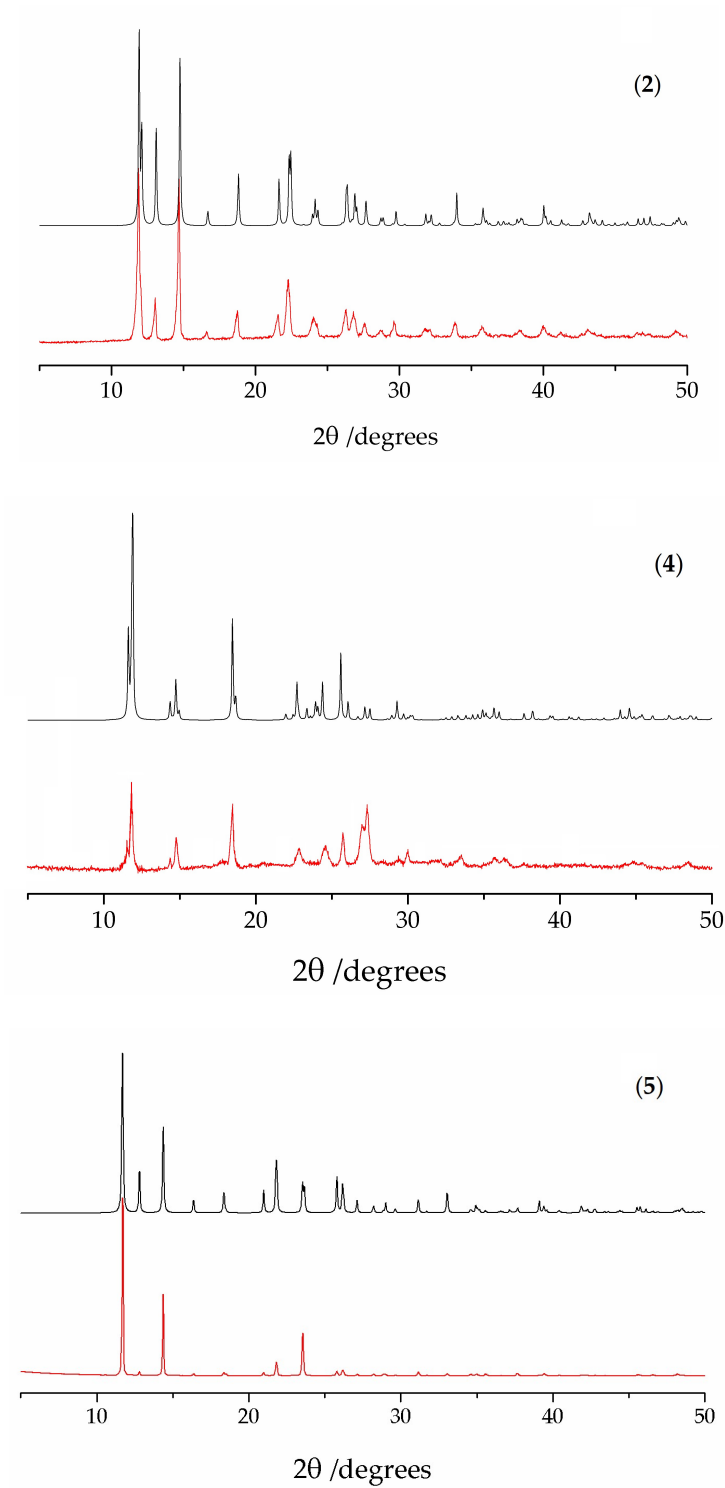**Figure S3.** FAB-MS spectra of complexes (**1**) (up) and (**3**) (down).

Figure S4. Powder XRD patterns for compounds (**2**), (**4**) and (**5**) (in red) shown in comparison with the simulated XRD from SC-XRD data (in black)
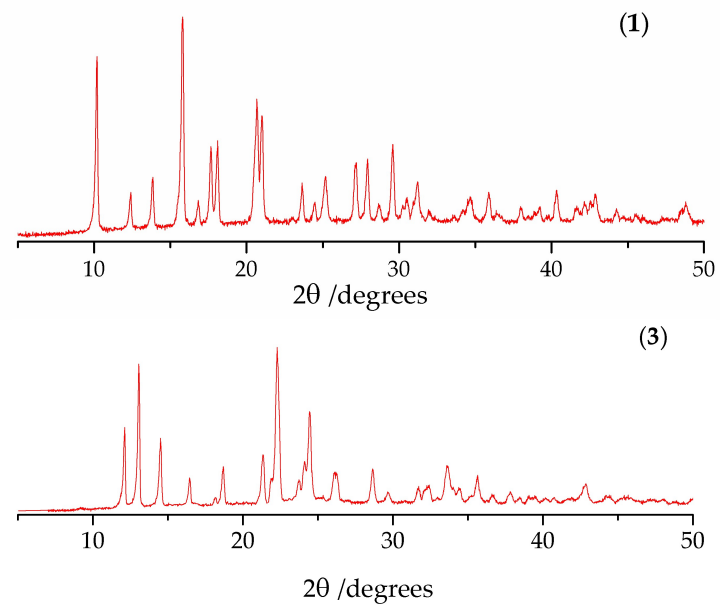
Figure S5. Powder XRD patterns for compounds (**1**) and (**3**)