

# Antiproliferative copper(II) complexes bearing mixed chelating ligands: structural characterization, ROS scavenging, antitumor activity and *in silico* studies

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**Table S1.** IR bands (cm<sup>-1</sup>) together with corresponding assignments.

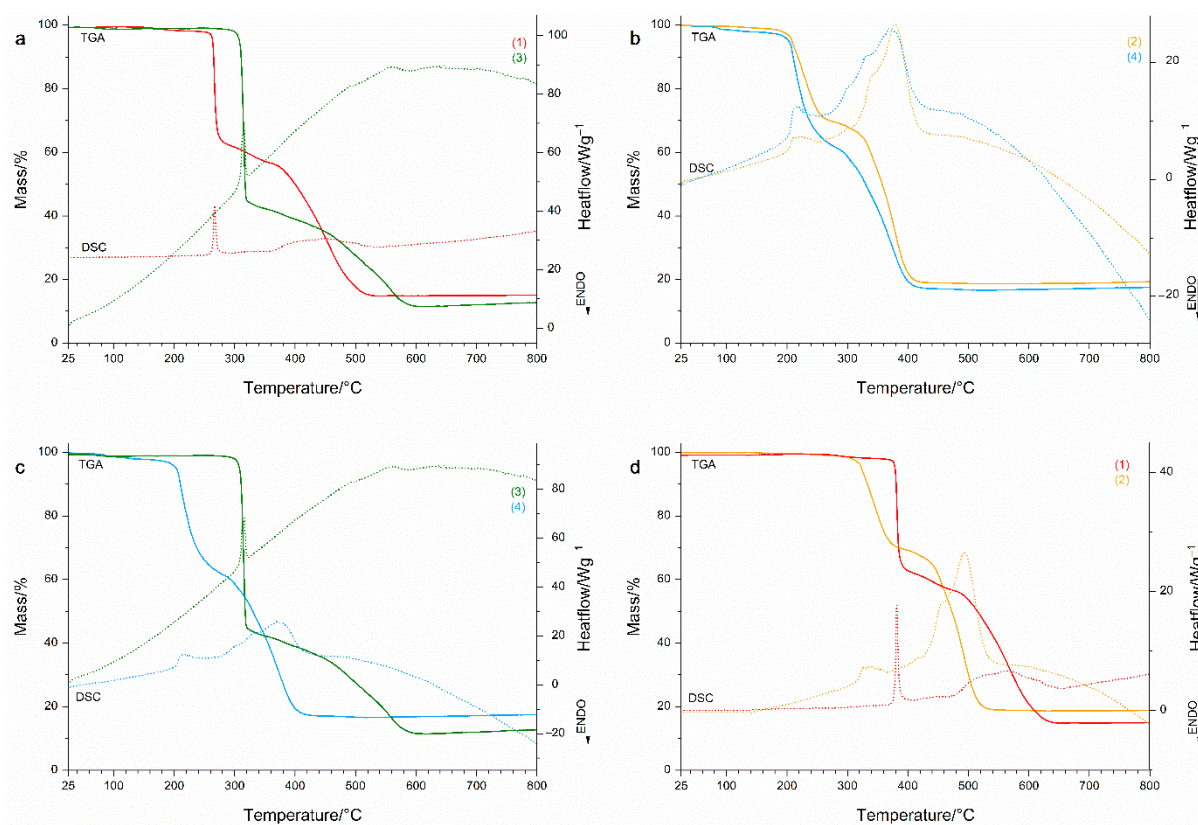
(1)	(2)	(3)	(4)	Assignments
-	3475m	-	-	v(H <sub>2</sub> O)
1615 m	1615 m	1605 m	1605 m	v(C=O)
1590 m	1590 m	1590 m	1590 m	v(C=N)
1560 s	1560 s	1560 m	1560 s	
-	1520 s 1320 m	-	1520 s 1315 s	v <sub>3</sub> (NO <sub>3</sub> )
1485 m	1485 m	1485 m	1485 m	v(C=C)
1450 m	1450 m	1450 m	1450 m	
1425 m	1425 m	1435 m	1435 m	
1105 vs 1065 s	1020 m	1090 vs	1025 m	v <sub>3</sub> (ClO <sub>4</sub> )/ v <sub>1</sub> (NO <sub>3</sub> )
960 m	-	-	-	v <sub>1</sub> (ClO <sub>4</sub> )
-	850 m	-	850 m	v <sub>2</sub> (NO <sub>3</sub> )
-	715 m	-	715 m	v <sub>4</sub> (NO <sub>3</sub> )
650 w 620 m	-	620 m	-	v <sub>4</sub> (ClO <sub>4</sub> )
445 w	445 w	450 w	460 w	v(Cu-N)
430 w	430 w	440 w	435 w	v(Cu-O)

s-strong; m-medium, w-weak.

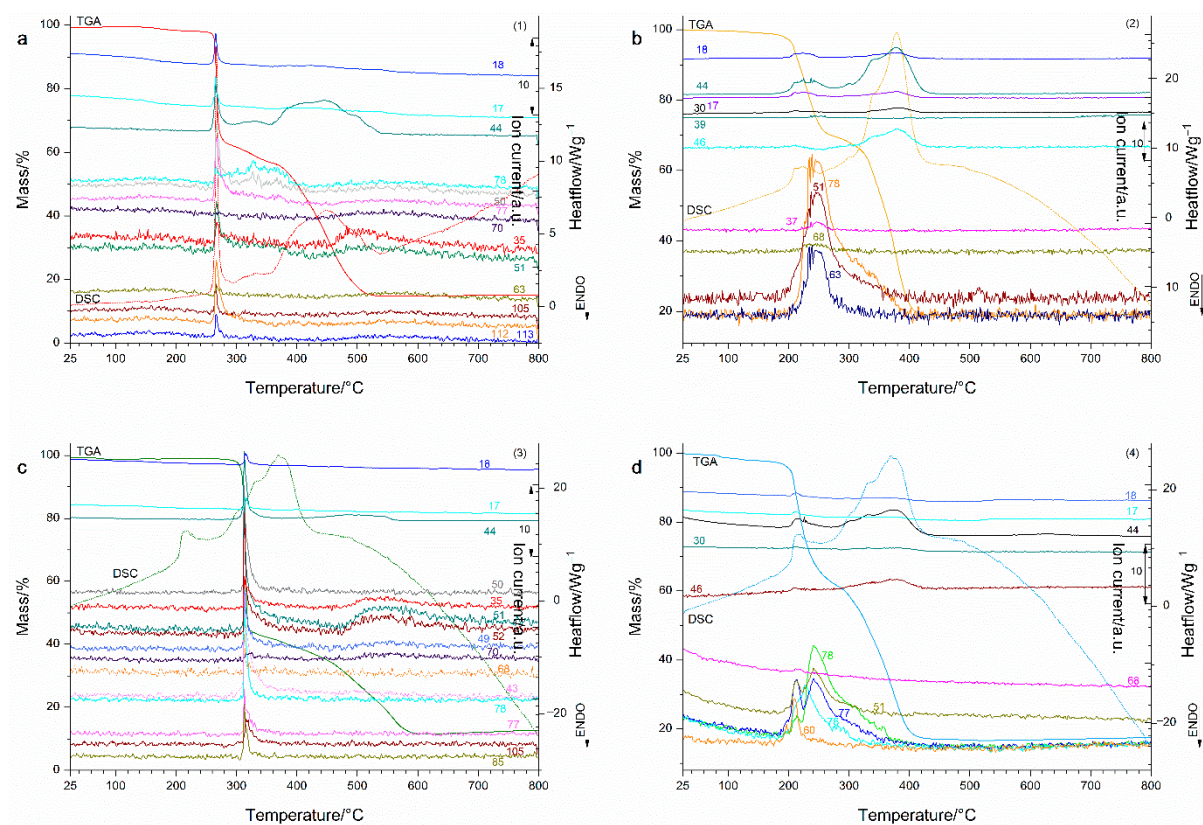
**Table S2.** Thermal data for complexes in air atmosphere. Representative mass peaks appear on Supplementary Figure S2.



Compound	Step	Thermal effect	Temperature range / °C	$\Delta m_{\text{exp}}$ / %	Identified product by EGA with corresponding $m/z$ values
(1)	1.	Exothermic	125-292	37.75	moieties from bzac ( $\text{C}_6\text{H}_5$ (77, 78), 105, (51, 50), moieties from phen ( $\text{C}_6\text{H}_{13}\text{N}_2$ (112, 113), 63, 50), perchlorate (Cl (35), $\text{CHCl}$ (49), $\text{ClO}$ (51, 52), $\text{H}_2\text{O}$ (17, 18), $\text{CO}_2$ (44)
	2.	Exothermic	292-352	5.07	moieties from bzac and phen (77, 78, 51, 50), $\text{H}_2\text{O}$ (17, 18), $\text{CO}_2$ (44)
	3.	Exothermic	352-569	41.77	perchlorate (Cl (35), $\text{CHCl}$ (49), $\text{ClO}$ (50, 51), $\text{Cl}_2$ (70)), $\text{H}_2\text{O}$ (17, 18), $\text{CO}_2$ (44), still some organic moiety
(2)	1.	Endothermic	25-155	2.96	$\text{H}_2\text{O}$ (17, 18)
	2.	Exothermic	155-214	7.73	moieties from bzac ( $\text{C}_4\text{H}_5\text{O}$ (68), $\text{C}_6\text{H}_5$ (77, 78), 51), $\text{H}_2\text{O}$ (17, 18), $\text{CO}_2$ (44)
	3.	Exothermic	214-304	23.99	moieties from bzac ( $\text{C}_4\text{H}_5\text{O}$ (68), $\text{C}_6\text{H}_5$ (77, 78), 51), moieties from phen ( $\text{C}_6\text{H}_{13}\text{N}_2$ (112, 113), 63, 50), nitrate ( $\text{NO}$ (30), $\text{NO}_2$ (46)), $\text{H}_2\text{O}$ (17, 18), $\text{CO}_2$ (44)
	4.	Exothermic	304-509	48.65	moieties from bzac ( $\text{C}_4\text{H}_5\text{O}$ (68), $\text{C}_6\text{H}_5$ (77, 78), moieties from phen ( $\text{C}_6\text{H}_{13}\text{N}_2$ (112, 113), 63, 50), nitrate ( $\text{NO}$ (30), $\text{NO}_2$ (46)), $\text{H}_2\text{O}$ (17, 18), $\text{CO}_2$ (44)
(3)	1.	Exothermic	251-320	54.36	moieties from bzac ( $\text{C}_4\text{H}_5\text{O}$ (68), $\text{C}_6\text{H}_5$ (77, 78), 105, 85, 43, (51, 50), moieties from bpy ( $\text{C}_5\text{H}_6\text{N}$ (78, 79), (51, 52, 50), perchlorate (Cl (35), $\text{CHCl}$ (49), $\text{ClO}$ (51, 52)), $\text{H}_2\text{O}$ (17, 18), $\text{CO}_2$ (44)
	2.	Exothermic	320-600	31.65	perchlorate (Cl (35), $\text{CHCl}$ (49), $\text{ClO}$ (51, 52), $\text{Cl}_2$ (70)), $\text{CO}_2$ (44)
(4)	1.	Exothermic	150-278	37.75	moieties from bzac ( $\text{C}_4\text{H}_5\text{O}$ (68, 69), $\text{C}_6\text{H}_5$ (77, 78), 60, 51), nitrate ( $\text{NO}$ (30), $\text{NO}_2$ (46)), $\text{H}_2\text{O}$ (17, 18), $\text{CO}_2$ (44)
	2.	Exothermic	278-304	4.70	moieties from bzac ( $\text{C}_6\text{H}_5$ (77, 78), 105, 51, 43) moieties from bpy ( $\text{C}_5\text{H}_6\text{N}$ (78, 79), (51, 52, 50), nitrate ( $\text{NO}$ (30), $\text{NO}_2$ (46)), $\text{H}_2\text{O}$ (17, 18), $\text{CO}_2$ (44)
	3.	Exothermic	304-337	11.29	still some organic moiety, nitrate ( $\text{NO}$ (30), $\text{NO}_2$ (46)), $\text{H}_2\text{O}$ (17, 18), $\text{CO}_2$ (44)
	4.	Exothermic	337-538	30.03	nitrate ( $\text{NO}$ (30), $\text{NO}_2$ (46)), $\text{H}_2\text{O}$ (17, 18), $\text{CO}_2$ (44)



**Figure S1.** TG-DSC graphs in air atmosphere from 25 °C to 600 °C in various combinations: **a)** complexes with perchlorate ligand, **b)** complexes with nitrate ligand, **c)** complexes with bpy ligand, and **d)** complexes with phen ligand.



**Figure S2.** TG/DSC-MS graphs of all complexes from 25 to 600 °C in air atmosphere: **a)** complex (1), **b)** complex (2), **c)** complex (3), and, **d)** complex (4).