Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Two Cu(II)-triadimenol complexes as potential fungicides: synergistic actions and DFT calculations

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Figure and table captions

Figure S1. UV-Vis spectra of two complexes and the ligand **L**.

Figure S2. EPR spectra of two complexes.

Figure S3. Thermal dependence of the X_MT product for complexes **1-2**.

Table S1. Selected structural parameters by X-ray and theoretical calculations for both complexes.

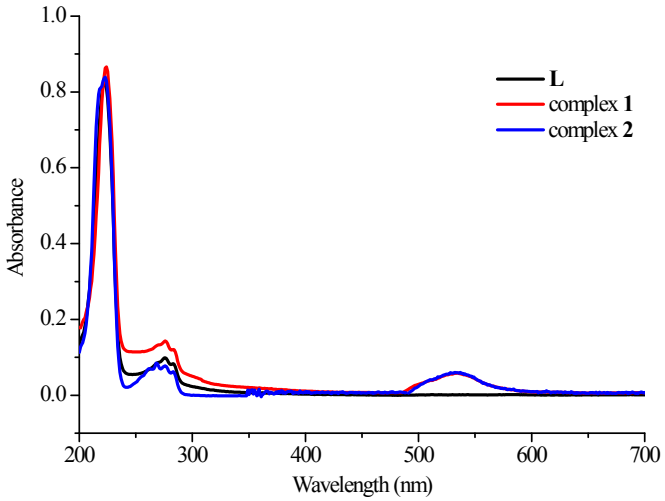

Fig. S1 UV-Vis spectra of two complexes and the ligand **L**.

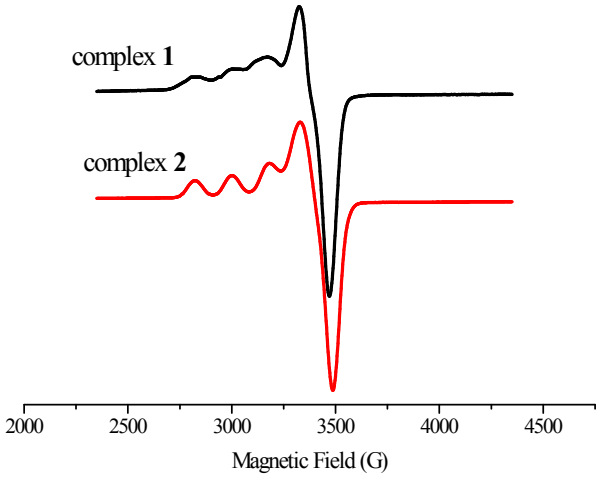

Fig. S2 EPR spectra of two complexes.

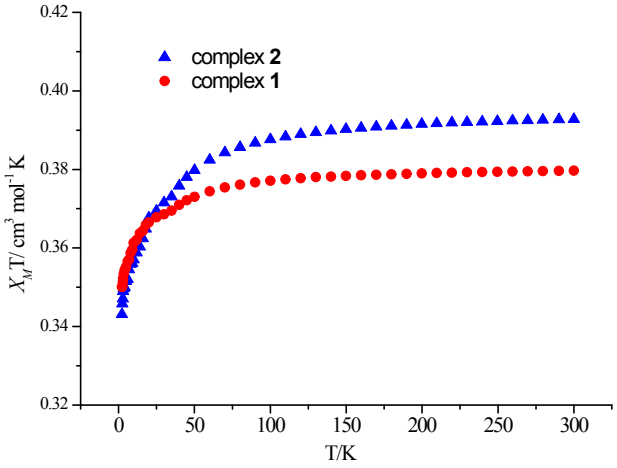

Fig. S3 Thermal dependence of the X_MT product for complexes **1-2**.

Table S1 Selected structural parameters by X-ray and theoretical calculations for both complexes.

	Complex **1**			Complex **2**	
	Expt.	Calcd.		Expt.	Calcd.
Bond lengths(Å)			Bond lengths(Å)		
Cu–N1	2.035(2)	2.127	Cu–N1	1.9950(18)	2.036
Cu–N4	2.030(2)	2.113	Cu–O1	2.6610(27)	2.783
Cu–O9w	2.392(2)	2.544	Cu–O2	1.9410(16)	1.992
C1–N1	1.323(4) .	1.333	C1–N1	1.351(3)	1.370
N1–C2	1.350(4)	1.349	N1–C2	1.320(3)	1.337
C2–N3	1.307(4)	1.365	C2–N2	1.324(3)	1.342
N3–N2	1.364(3)	1.326	N2–N3	1.354(3)	1.368
Bond angles (º)			Bond angles (º)		
N1–Cu–N1i	180.00(13)	180.00	N1–Cu–N1i	180.00(12)	180.00
N4–Cu–N4i	180.00(18)	180.00	O2–Cu–O2i	180.00(13)	180.00
O9w–Cu–O9wi	180.00(11)	180.00	O1–Cu–O1i	180.00(1)	180.00
N1–Cu–N4	91.01(9)	95.789	N1–Cu–O2	89.13(7)	90.211
N1–Cu–N4i	88.99(9)	90.277	N1–Cu–O1	93.598(73)	95.789

Symmetry code: complex **1** (i) $-x + 2, -y + 1, -z$; complex **2** (ii) $-x + 1, -y + 1, -z + 2$.