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First example of a click-reaction on the aminate copper complexes: effect of reaction parameters

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Table S1 Crystallographic data and refinement parameters of complexes **1** and **2**

Parameter/Compound	**1**	**2**
Formula of the complex	***cis*-[Cu(phen)$_2$(mtz)$_2$]·H$_2$O**	**[Cu(phen)(μ-CN)]$_n$**
Formula	$C_{28}H_{24}CuN_{12}O$	$C_{26}H_{16}Cu_2N_6$
Molecular weight	608,12	539,53
Crystal system	monoclinic	monoclinic
Space group	C 2/c	P 2_1/c
a, Å	9.5063(3)	18.4775(8)
b, Å	15.4116(6)	8.3433(3)
c, Å	17.5253(7)	16.5648(8)
α, deg	90	90
β, deg	93.945(3)	110.044(5)
γ, deg	90	90
V, Å^3	2561.5	2399.01(19)
Z	4	4
d_{calc}, g/cm^3	1.577	1.494
F(000)	1252	1088
μ, mm^{-1}	0.903	2.389
Reflection indices	-11 ≤ h ≤ 12 -20 ≤ k ≤ 17 -16 ≤ l ≤ 22	-22 ≤ h ≤ 22 -10 ≤ k ≤ 6 -18 ≤ l ≤ 20
$2\theta_{max}$, deg	55.00	140.00
Total/independent/ $I > 2\sigma(I)$ reflection number	8250/2947/2630	14089/4560/3919
R_{int}	0.0349	0.0290
Number of variables	196	309
$\Delta\rho_{max}$, $\Delta\rho_{min}$, $\bar{e}$/ Å^3	0.414, -0.349	0.945, -0.730
Goodness of fit	1.038	1.035
R Factors [reflections with $I > 2\sigma(I)$]: R_1 wR_2	 0.0305 0.0711	 0.0409 0.1047
R Factors (all reflections): R_1 wR_2	 0.0366 0.0742	 0.0472 0.1094

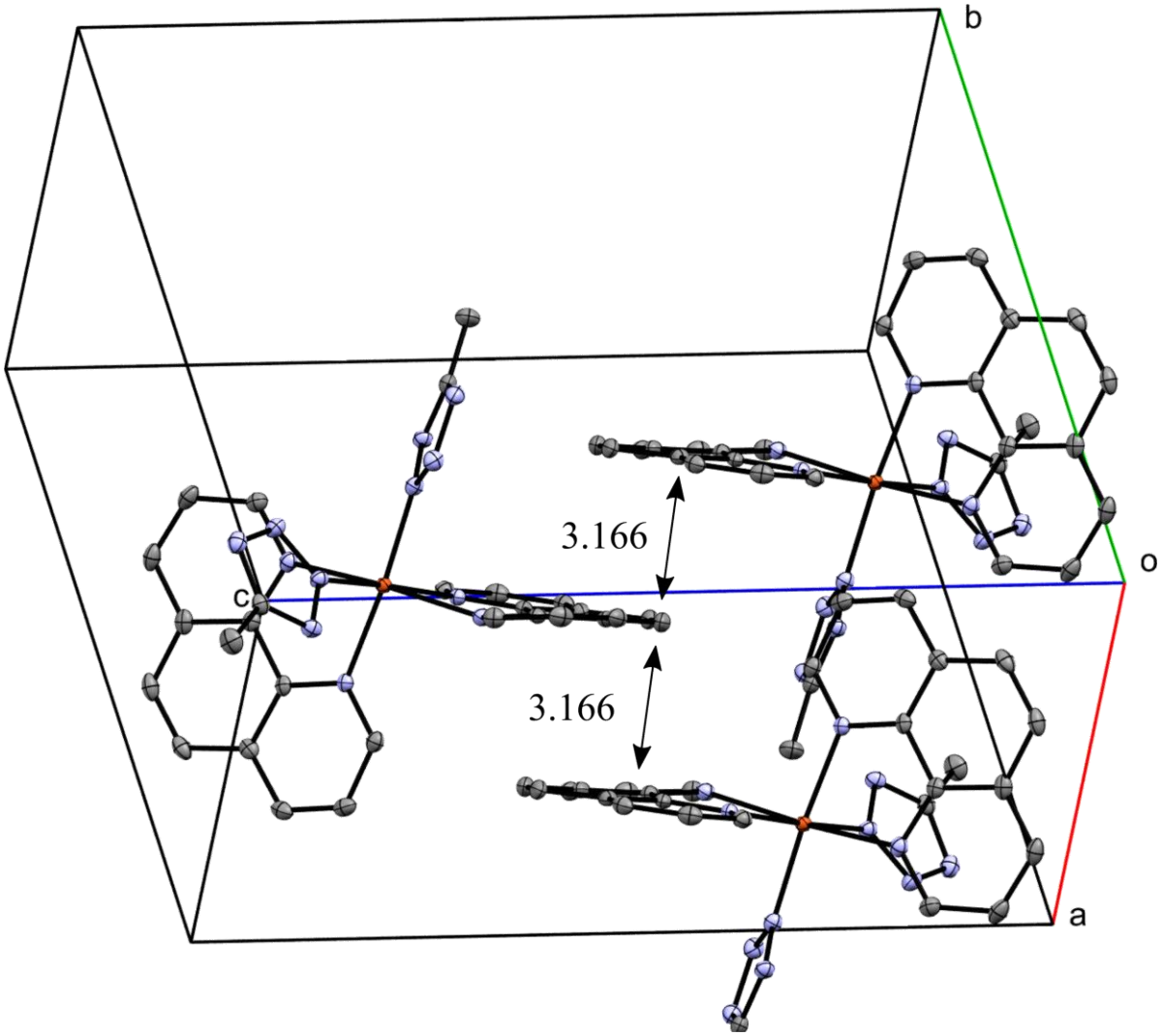

Figure S1 Fragment of crystal structure **1** with p–p stacking of Phen ligand (distances are given in Å).

Table S2 Selected bond lengths (Å) in **1** and some known complexes of copper(II) with tetrazole.

Compound	Coordination number	Cu–$N_{(Phen\ or\ Dipy)}$	Cu–$N_{tetrazole}$, coordination atom			Reference
			1	2	3	
1	6	2.074; 2.309	-	2.016	-	This work
$[Cu_2(Dipy)_2(\mu_2\text{-Ph-tz})_2(Ph\text{-tz})_2]$	5	2.008; 2.029	-	2.010	2.196	[23]
$[Cu_2(Dipy)_2(\mu_2\text{-(FeCp-tz)})_2(FeCp\text{-tz})_2]$	5	2.011; 2.037	-	2.024	2.182	[24]
$[Cu_2(Dipy)_2(\mu_2\text{-(CN-tz)})_2(CN\text{-tz})_2]$	5	2.013; 2.037	-	2.004	2.371	[25]
catena-[Cu(Dipy)(μ_2-(CN-tz))(CN-tz)]	5	2.003; 2.023	2.016	1.999	-	[25]
$[Cu_2(Dipy)_2(N_3)_2(\mu_2\text{-Pyz-tz})_2]$	6	2.015; 2.042	2.037	-	2.302	[26]
$[Cu_2(Dipy)_2(\mu_2\text{-Ph-dtz})_2]$	5	2.025; 2.027	1.966 1.995	-	2.197	[27]

Dipy = 2,2'-bipyridine; Ph-tz = 5-Phenyltetrazole; FeCp-tz = 5-(1-ferrocenyl)tetrazole; CN-tz = 5-cyanotetrazole; Pyz-tz = 5-(Pyrazin-2-yl)tetrazole; Ph-dtz = 5,5'-(1,2-phenylene)ditetrazole

Table S3 Selected bond lengths (Å) in **2** and similar complexes of copper(II).

Compound	Cu–$N_{(Phen)}$	Cu–$N_{(CN)}$	Cu–$C_{(CN)}$	C≡N	Reference
2	2.133, 2.119, 2.104, 2.107	1.942, 1.964	1.938, 1.939	1.145, 1.148	This work
$[Cu_3(Phen)_2(\mu_2\text{-CN})_3]_n$	2.104, 2.017, 2.124, 2.070	1.956, 1.926	1.896, 1.848	1.155, 1.150	[28]
$[Cu_3(Phen)_2(\mu_2\text{-CN})_3]_n$	2.086, 2.155, 2.021, 2.111	1.970, 1.920	1.852, 1.897	1.155, 1.147	[29]
$[Cu(Phen)(\mu_2\text{-CN})]_n$	2.144, 2.118, 2.144, 2.084	1.934, 1.934	1.898, 1.898	1.143, 1.143	[16]
$[Cu(Phen)(\mu_2\text{-CN})]_n{\cdot}CH_3OH$	2.114, 2.120, 2.104, 2.094	1.927, 1.940	1.911, 1.913	1.157, 1.160	[17]
$[Cu(Phen)(\mu_2\text{-CN})]_n{\cdot}C_2H_5OH$	2.129, 2.142, 2.126, 2.107	1.921, 1.944	1.910, 1.910	1.167, 1.153	[18]

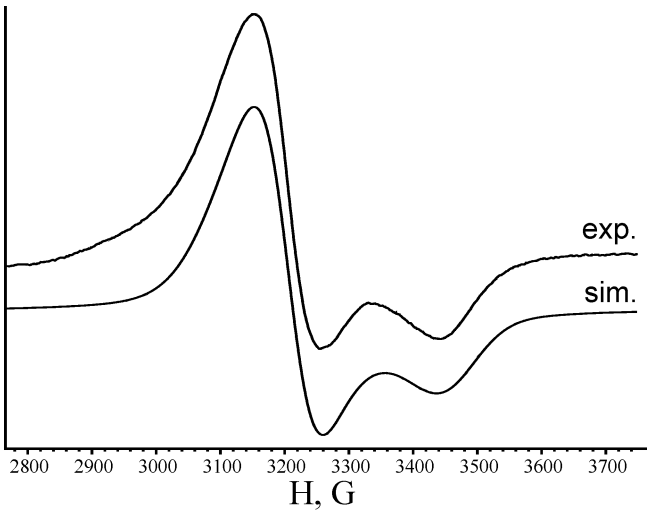

Figure S2 The X-band EPR spectrum of complex **1** in solid state at 298 K (*exp.*) and its simulation (*sim.*) performed using the WINEPR Simfonia 1.25 program (Bruker).

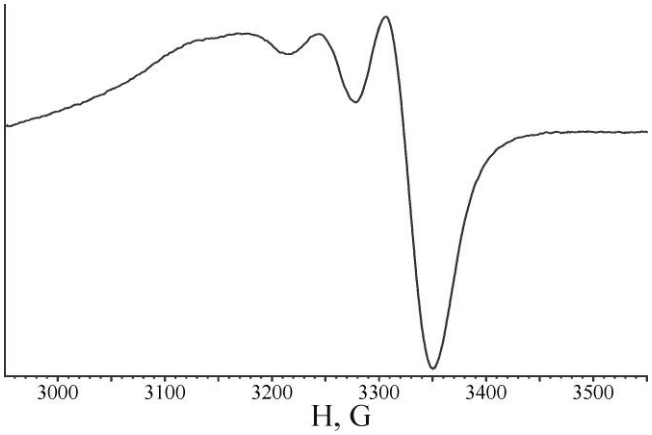

Figure S3 The isotropic X-band EPR spectrum of complex **1** in solution (DMSO, 298K).