Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Table S1. Quantum chemical parameters of complexation of AZOs and Cu^{2+} (2:1 stoichiometry) calculated with b3lyp/6-31g(d,p)//Lanl2dz.

Complexation		Binding Energy (kcal/mol)	Distance (Å)			Angle (°) *	
			Cu^{2+}... N	Cu^{2+}... $O_{carboxyl}$	Cu^{2+}... $O_{methoxy}$	$\angle NCu^{2+}O_{carboxyl}$	$\angle NCu^{2+}O_{methoxy}$
1+Cu^{2+}+1	a1	-219.327	2.161 and 2.170	1.919 and 1.938	2.742 and 2.877	81.0 and 84.4	65.1 and 63.2
	a2	-223.606	2.115 and 2.128	1.954 and 1.971	2.457 and 2.577	82.8 and 83.9	73.5 and 75.7
	a3	-216.900	2.162 and 2.165	1.946 and 1.947	2.862 and 2.891	81.9 and 82.0	63.0 and 63.6
2+Cu^{2+}+2	b1	-206.043	2.166 and 2.208	1.933 and 1.935	--	83.5 and 96.1	--
	b2	-213.857	2.150 and 2.150	1.914 and 1.914	--	84.3 and 84.3	--
	b3	-204.890	2.189 and 2.228	1.929 and 1.931	--	83.0 and 96.5	--
	b4	-213.894	2.151 and 2.152	1.914 and 1.914	--	84.3 and 84.4	--

* There were total four $\angle NCu^{2+}O_{carboxyl}$ angles, only two smaller values were recorded here, and the same for $\angle NCu^{2+}O_{methoxy}$.

Table S2. Binding energies of complexation of AZOs 1:1 stoichiometry chelated to Cu^{2+} calculated with b3lyp/6-31g(d,p)//Lanl2dz.

Complexation	Binding Energies (kcal/mol)		
	ΔE_1	ΔE_2	ΔE
$1+Cu^{2+}+2Cl^-$	-119.263	-32.925	-241.589
$1+Cu^{2+}+2H_2O$	-160.862	-32.421	-248.296
$2+Cu^{2+}+Cl^-$	-127.272	-27.833	-224.407
$2+Cu^{2+}+H_2O$	-174.463	-23.001	-222.576

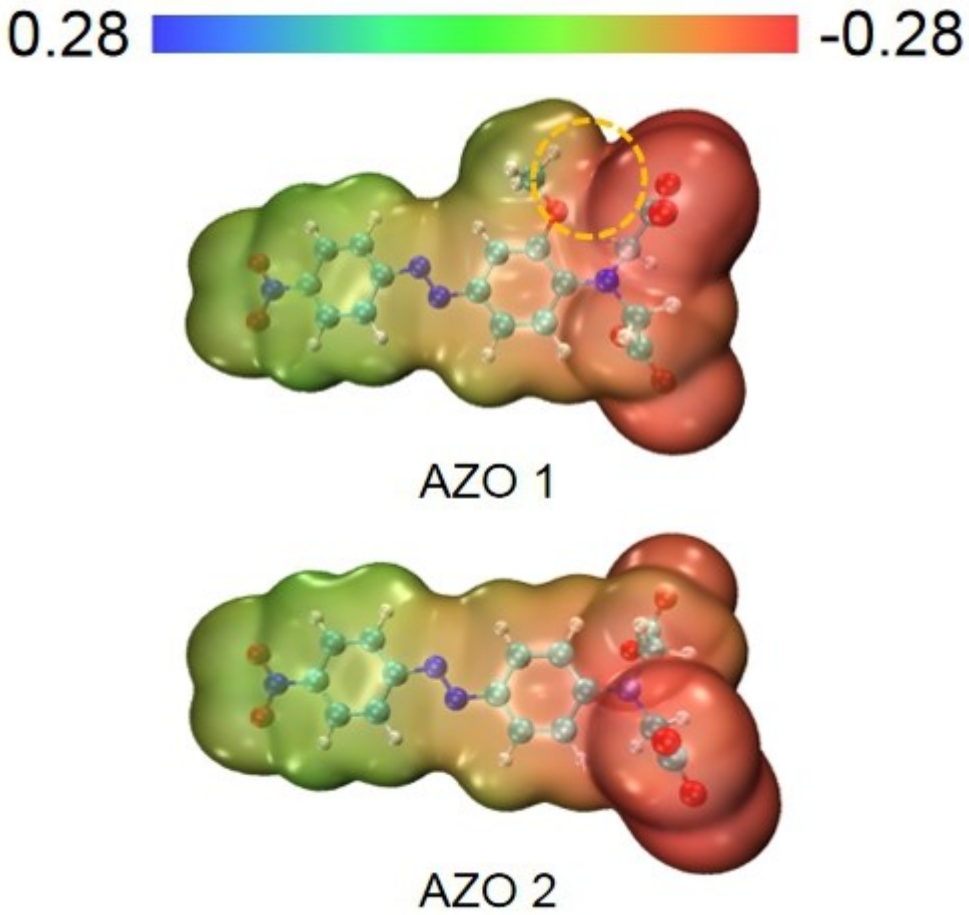

Figure S1. The mapped electrostatic potential surfaces of AZO 1 and AZO 2.

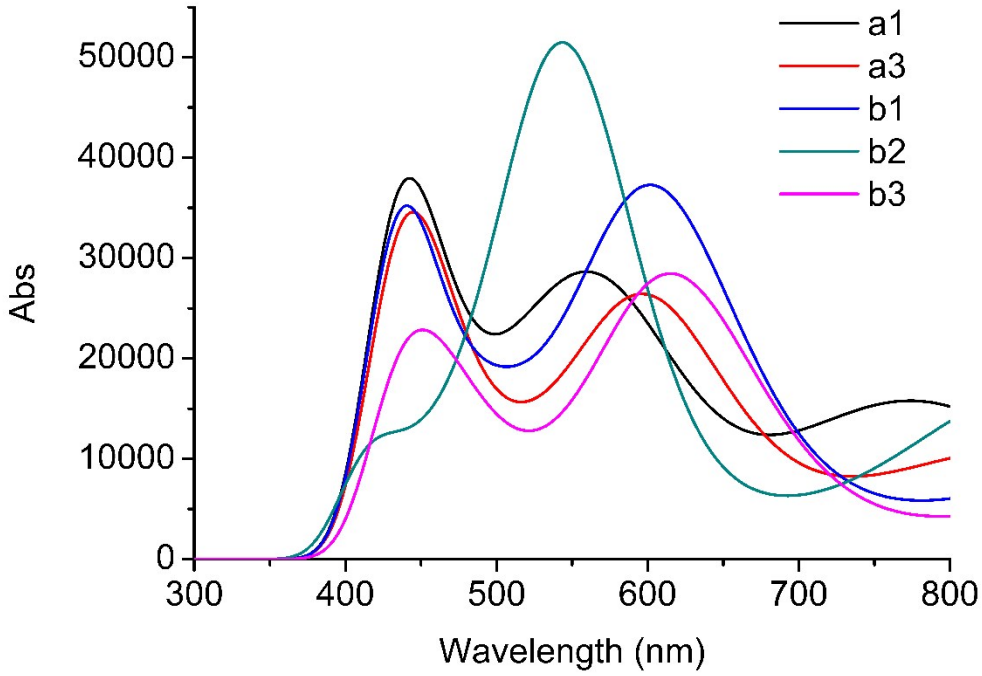

Figure S2. Calculated UV-vis spectra of complexztion of 2:1 stoichiometry for AZOs and Cu^{2+} of a1, a3, b1, b2 and b3 at the levels of td-b3lyp/6-31g(d,p)//Lanl2dz.

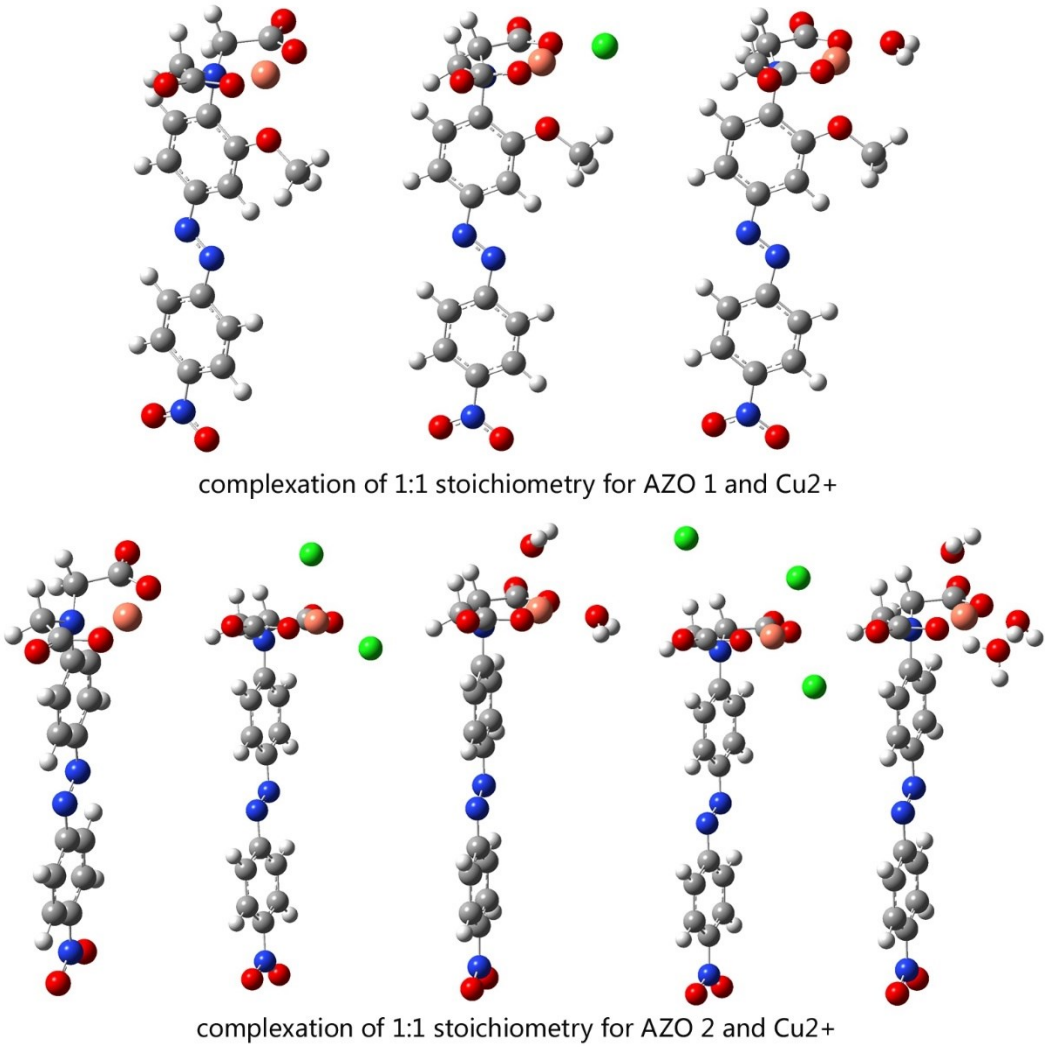

Figure S3. Other optimized structures of 1:1 stoichiometry for AZOs and Cu^{2+}, except the complexation in Figure 5, calculated at the levels of b3lyp/6-31g(d,p)//Lanl2dz.

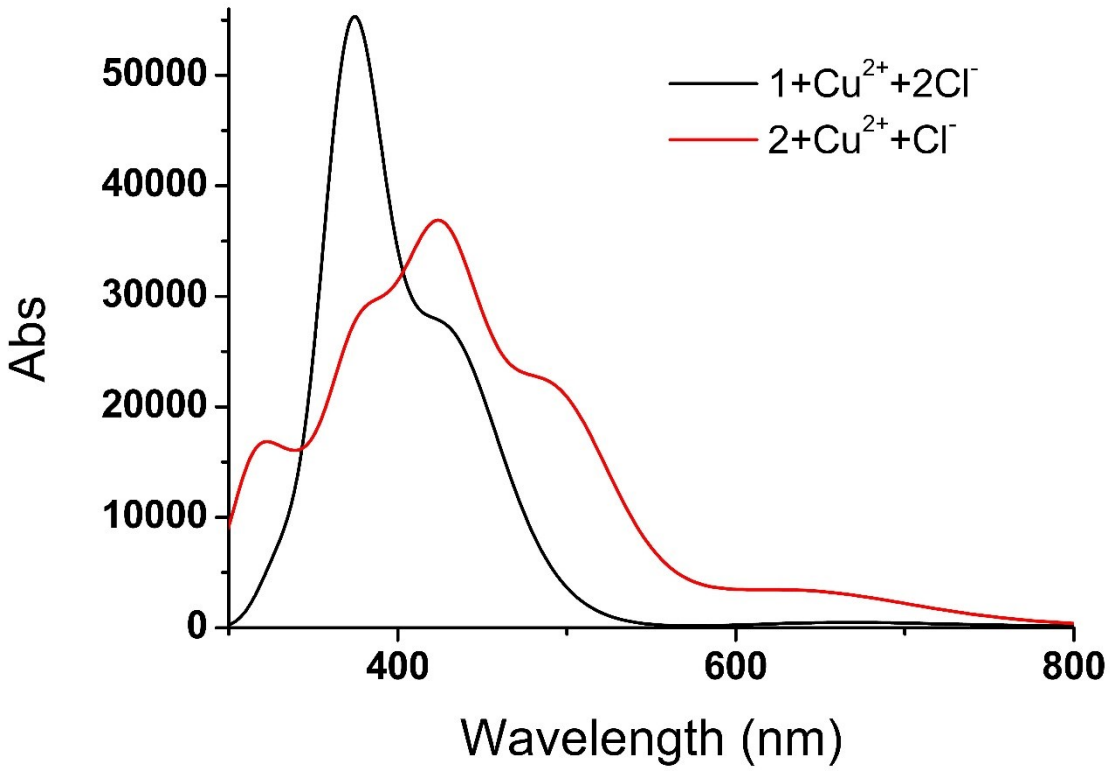

Figure S4. Calculated UV-vis spectra of $1+Cu^{2+}+2Cl^-$ and $2+Cu^{2+}+Cl^-$.