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Supplementary material

SUPPLEMENTARY MATERIAL TO

(*E*)-4-(((2-Amino-5-chlorophenyl)imino)methyl)-5-(hydroxymethyl)-2-methylpyridin-3-ol and its Cu(II) complex: Synthesis, DFT calculations and AIM analysis

MORTEZA YAVARI, S. ALI BEYRAMABADI*, ALI MORSALI and MOHAMMAD REZA BOZORGMEHR

Department of Chemistry, Mashhad Branch, Islamic Azad University, Mashhad, Iran

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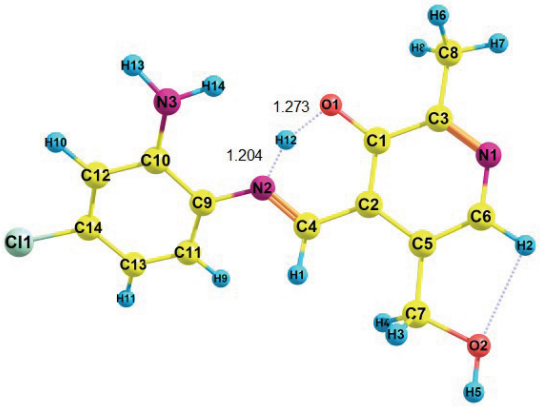

Fig. S-1. The M062X optimized geometry of the TSEnol-Keto of the *meta* isomer.

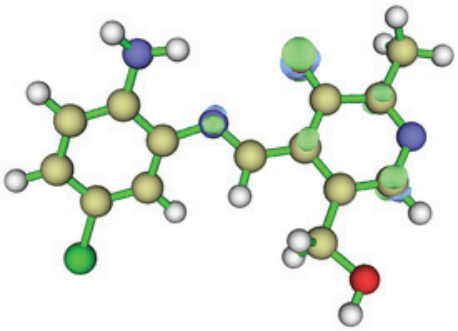

Fig. S-2. Optimized geometry and the isosurface Fukui map of $\mathbf{L}^{-}$.

* Corresponding author. E-mails: beiramabadi6285@mshdiau.ac.ir; beiramabadi@yahoo.com

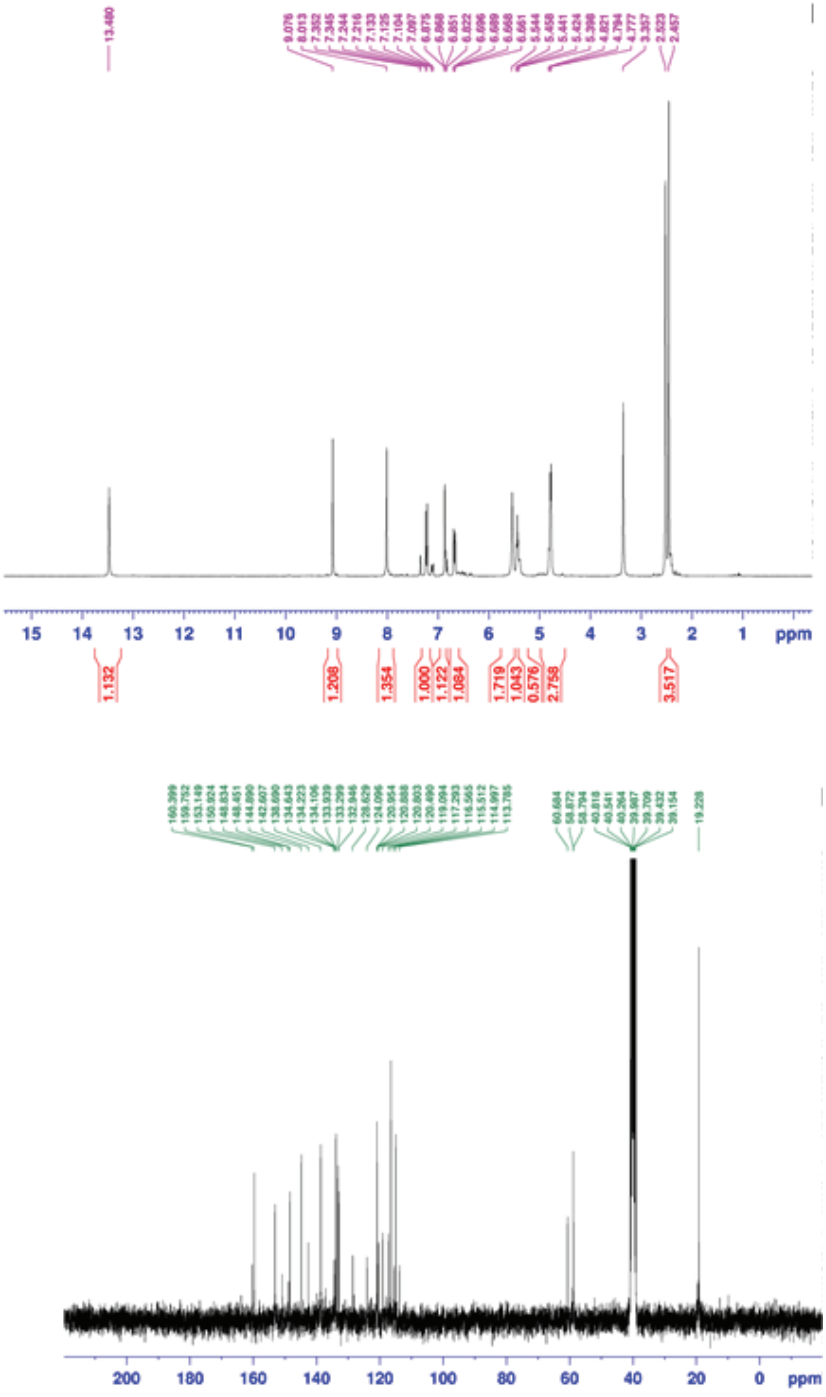

Fig. S-3. The ^{1}H- and ^{13}C-NMR spectra of the **HL** Schiff base.

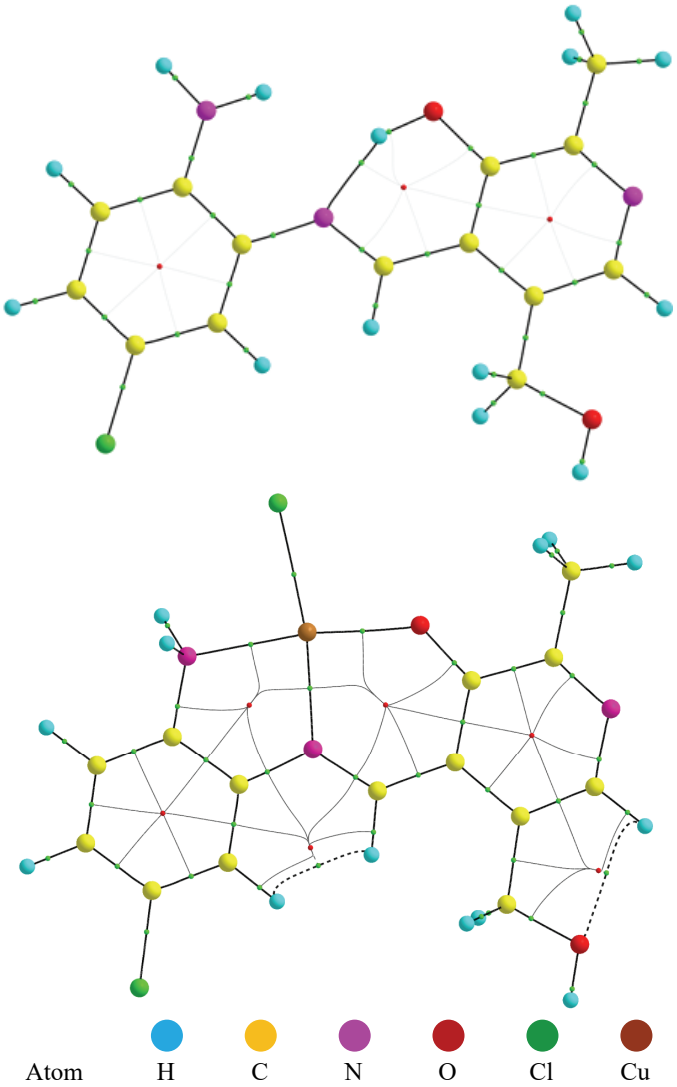

Fig. S-4. The QTAIM molecular graphs of the **HL** Schiff base and the [Cu(**L**)Cl] complex (small green and red spheres correspond to the BCPs and RCPs, respectively).

TABLE S-I. The elemental analysis of the investigated compounds

Species	Content, %								Chemical formula
	Calculated				Experimental				
	C	H	N	Metal	C	H	N	Metal	
HL	57.64	4.84	14.40	–	57.34	4.76	15.01	–	$C_{14}H_{14}ClN_3O_2$
[Cu(**L**)Cl]	43.15	3.36	10.78	16.31	43.52	3.48	10.46	17.02	$C_{14}H_{13}Cl_2CuN_3O_2$

TABLE S-II. Relative electronic energies (E+ZPE) for the investigated species of the **HL** Schiff base

Species	E+ZPE / kJ mol^{-1}		ΔG / kJ mol^{-1}
	Methanol solution	Gas phase	Methanol solution
Enol tautomer of the *meta* isomer	0	0	0
Keto tautomer of the *meta* isomer	28.85	35.07	24.59
Enol tautomer of the *para* isomer	19.02	21.06	20.94
Keto tautomer of the *para* isomer	25.14	31.92	28.63
TSEnol-Keto	163.01	160.54	131.02

TABLE S-III. Important experimental and the DFT-computed IR vibrational frequencies (VF) of the **HL** Schiff base (enol tautomer of the *meta* isomer) and [Cu(**L**)Cl] complex

Experimental frequencies		Calculated frequencies				Vibrational assignment
		HL		[Cu(**L**)Cl]		
HL	[Cu(**L**)Cl]	ν / cm^{-1}	Intensity km mol^{-1}	ν / cm^{-1}	Intensity km mol^{-1}	
–	547 (*m*)	–	–	540	29	υ_{asym}(Cu–N, Cu–O)
–	640 (*w*)	–	–	625	5	υ_{sym}(Cu–N, Cu–O)
765 (*m*)	767 (*m*)	750	12	727	11	Breathing of the aromatic rings
809 (*m*)	–	802	54	–	–	δ_{op}(H12)
846 (*w*)	851 (*w*)	846	20	851	27	δ_{op}(aromatic hydrogens)
912 (*w*)	915 (*w*)	885	56	907	86	υ(C13–Cl1)
1032 (*vs*)	1027 (*s*)	1060	68	1149	271	υ(C7–O2)
1208 (*m*)	1188 (*m*)	1174	85	1171	186	υ(C9–N2)
1298 (*m*)	1262 (*m*)	1278	94	1256	139	υ(C10–N3)+ υ(Ar–C)
1380 (*vs*)	1416 (*vs*)	1389	218	1378	156	υ(C1–O1)
1471 (*m*)		1457	127	1450	234	υ(C9–N2)
1521 (*m*)	1507 (*m*)	1578	154	1484	191	υ_{asym}(C=C) of the benzene ring
		1559	117	1532	192	υ_{sym}(C=C) of the benzene ring
		1572	100	1554	91	υ(C=N, C=C) of the pyridine ring + υ(C4–N2)
1617 (*vs*)	1605 (*vs*)	1594	140	1595	28	υ(C=N, C=C) of the pyridine ring
		1604	16	1602	331	υ(C4=N2)
2746 (*m*)	2741 (*s*)	2853	40	2882	47	υ_{sym}(C–H) of –CH_2– groups
2840 (*s*)	2838 (*s*)	2876	30	2911	27	υ_{asym}(C–H) of –CH_2– groups
2919 (*s*)	2918 (*s*)	2914	19	2953	7	υ_{sym}(C–H) of the methyl groups

3110 (*vs*, *br*)	3096 (v*s*, *br*)	2956	33	3039	10	υ(C4–H1)
		2959	14	3061	9	υ_{asym}(C–H) of the methyl groups
		3088–3046	3	3125–3087	2	υ_{asym}(C–H) of the aromatic hydrogens
		3129	467	–	–	υ(O1–H12)
3463 (*m*, *br*)	3362 (*s*)	3439	26	3368	58	υ_{sym}(H–N–H) of the –NH_2 amine group
	3444 (*s*)	3541	35	3427	57	υ_{asym}(H–N–H) of the –NH_2 amine group
		3708	59	3773	79	υ(O2–H5)

TABLE S-IV. Important topological parameters of the investigated

Bond	$\rho(r)$ / ea_0^{-3}	$\nabla^2\rho$	V_b / kJ mol^{-1}	G_b / kJ mol^{-1}	H_b / kJ mol^{-1}	$-G_b/V_b$
HL Schiff base						
C1–O1	0.296455	–0.29584	–2069.64	937.82	–1131.82	0.45
O1–H12	0.328394	–2.3074	–1861.35	174.14	–1687.21	0.09
N2···H12	0.048682	0.117582	–123.01	100.06	–22.95	0.81
C4–N2	0.360837	–0.74918	–2447.96	978.35	–1469.62	0.40
C9–N2	0.288529	–0.79631	–1405.12	441.47	–963.65	0.31
C10–N3	0.300363	–0.85216	–1520.38	480.79	–1039.59	0.32
C7–O2	0.253926	–0.44675	–1481.29	594.16	–887.12	0.40
O2–H5	0.36575	–2.53727	–2045.54	190.86	–1854.68	0.09
O2···H2	0.015016	0.075301	–31.9744	40.69	8.72	1.31
C13–Cl1	0.189228	–0.26237	–505.52	166.74	–338.78	0.33
[Cu(**L**)Cl] complex						
C1–O1	0.344817	0.072805	–2945.70	1496.72	–1448.98	0.51
C4–N2	0.35068	–0.58679	–2706.94	1161.08	–1545.86	0.43
C9–N2	0.292404	–0.91341	–1479.89	440.46	–1039.43	0.30
C10–N3	0.271821	–0.80724	–1285.78	378.22	–907.56	0.29
C7–O2	0.261951	–0.45338	–1703.82	703.26	–1000.56	0.41
O2–H5	0.353374	–1.87394	–1576.75	173.96	–1402.79	0.11
C13–Cl1	0.199477	–0.29389	–545.37	176.33	–369.04	0.32
Cu–O1	0.084756	0.630332	–409.91	411.63	1.72	1.00
Cu–N2	0.076368	0.468496	–316.97	312.09	–4.88	0.98
Cu–N3	0.068587	0.403737	–264.16	264.45	0.29	1.00
Cu–Cl2	0.065415	0.292258	–217.09	204.37	–12.72	0.94
O2···H2	0.015985	0.076722	–35.07	42.69	7.62	1.22