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Influence of metal ions (Zn^{2+}, Cu^{2+}, Ca^{2+}, Mg^{2+} and Na^{+}) on the water coordinated neutral and zwitterionic L-Histidine dimer

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Table S1

Electron density (ρ), Laplacian of electron density ($\nabla^2\rho$) and ellipticity (ε) and total electron energy density H(r) all values in (a.u) obtained from gas phase.

Structure	Bond Type(Å)	ρ		$\nabla^2\rho$		ε		H(r)	
		Neutral	Zw	Neutral	Zw	Neutral	Zw	Neutral	Zw
Zn^{2+}	N25-Zn	0.08184	0.07002	0.31358	0.25825	0.04589	0.04253	-0.017765	-0.01443
	N14-Zn	0.08183	0.06992	0.31349	0.25766	0.04591	0.04257	-0.0177675	-0.01441
	O6-Zn	0.05248	0.06784	0.24809	0.35878	0.03973	0.01928	-0.0057375	-0.00686
	O38-Zn	0.05249	0.06785	0.24814	0.35893	0.03975	0.01988	-0.005735	-0.00686
	O21-Zn	0.0516	0.05122	0.24899	0.24843	0.06314	0.06744	-0.0056625	-0.00562
	N2...H5-O8	0.04113	0.05483	0.10888	0.14736	0.11686	0.08041	-0.00384	-0.00724
	N41...H44-O40	0.04114	0.0551	0.1089	0.14757	0.11676	0.07961	-0.003845	-0.0074
Cu^{2+}	N25-Cu	0.08907	0.08234	0.37889	0.35075	0.02667	0.02274	-0.0163875	-0.01389
	N14-Cu	0.089	0.08234	0.37942	0.35076	0.02657	0.02273	-0.016335	-0.01389
	O6-Cu	0.06631	0.07682	0.38086	0.45654	0.09500	0.07637	-0.002595	-0.00382
	O38-Cu	0.06632	0.07682	0.38087	0.45656	0.09497	0.07640	-0.0025925	-0.00382
	O21-Cu	0.03433	0.03089	0.14514	0.12866	0.06816	0.08126	-0.003675	-0.00298
	N2...H5-O8	0.04322	0.05421	0.1102	0.14791	0.10834	0.08359	-0.00487	-0.00684
	N41...H44-O40	0.04325	0.05421	0.11016	0.14791	0.10826	0.08358	-0.00488	-0.00684
Ca^{2+}	N25-Ca	0.03393	0.03017	0.1461	0.13004	0.09717	0.08630	0.003095	0.00328
	N14-Ca	0.03594	0.03293	0.15635	0.14485	0.09487	0.08293	0.0031075	0.003423
	O6-Ca	0.03901	0.04674	0.22849	0.29048	0.08512	0.00293	0.0071325	0.00765
	O38-Ca	0.04113	0.04161	0.24886	0.23207	0.00735	0.07204	0.007565	0.006248
	O21-Ca	0.03296	0.03547	0.18327	0.1989	0.13935	0.13352	0.0061875	0.006325
	N2...H5-O8	0.04558	0.0522	0.11137	0.14595	0.09636	0.08857	-0.0061075	-0.00577
	N41...H44-O40	0.05005	0.03751	0.11111	0.12861	0.08083	0.15557	-0.0086925	0.000642
Mg^{2+}	N25-Mg	0.0355	0.03269	0.04728	0.1981	0.04874	0.03424	0.00647	0.006385
	N14- Mg	0.0355	0.03269	0.04728	0.1981	0.04874	0.03425	0.00647	0.006385

	O6- Mg	0.03688	0.04258	0.06252	0.36472	0.05486	0.03985	0.0130025	0.01489
	O38- Mg	0.03688	0.04258	0.06252	0.36472	0.05488	0.03985	0.013	0.01489
	O21- Mg	0.03224	0.03108	0.05139	0.23987	0.07184	0.08053	0.011015	0.010718
	N2...H5-O8	0.04711	0.05555	0.11157	0.14942	0.09171	0.07823	-0.0069575	-0.00756
	N41...H44-O40	0.04711	0.05555	0.11157	0.14942	0.09171	0.07823	-0.0069575	-0.00756
Na^+	N25-Na	0.01922	*	0.10856		0.04873		0.00468	
	N14-Na	0.01924		0.10873		0.04871		0.0046825	
	O6-Na	0.01807		0.12204		0.04271		0.00588	
	O38-Na	0.01805		0.12178		0.04283		0.005865	
	O21-Na	0.01931		0.12847		0.12195		0.0059175	
	N2...H5-O8	0.04084		0.11306		0.11313		-0.003515	
	N41...H44-O40	0.04079		0.11301		0.11337		-0.0034875	

***Data not available**

Table S2

Natural charges (in e) and dipole moment (Debye) of the complexes calculated in gas phase at B3lyp/6-311G level**

Structure	$Zn^{2+}(His)_2.H_2O$	$Cu^{2+}(His)_2.H_2O$	$Ca^{2+}(His)_2.H_2O$	$Mg^{2+}(His)_2.H_2O$	$Na^{+}(His)_2.H_2O$	$Zn^{2+}(His)_2.H_2O$	$Cu^{2+}(His)_2.H_2O$	$Ca^{2+}(His)_2.H_2O$	$Mg^{2+}(His)_2.H_2O$	$Na^{+}(His)_2.H_2O$
Metal	1.700	1.511	1.608	1.426	0.718	1.718	1.517	1.677	1.463	0.734
	(1.714)*	(1.500)	(1.592)	(1.417)	$	(1.724)	(1.517)	(1.640)	(1.424)	$
ΔQ	0.300	0.777	0.371	0.574	0.282	0.282	0.483	0.323	0.537	0.266
	(0.286)	(0.500)	(0.408)	(0.583)		(0.276)	(0.483)	(0.360)	(0.576)	
N25	-0.732	-0.665	-0.654	-0.650	-0.552	-0.719	-0.666	-0.633	-0.651	-0.572
	(-0.702)	(-0.654)	(-0.632)	(-0.637)		(-0.697)	(-0.599)	(-0.618)	(-0.633)	
N14	-0.732	-0.664	-0.662	-0.650	-0.551	-0.719	-0.666	-0.643	-0.651	-0.572
	(-0.702)	(-0.654)	(-0.635)	(-0.637)		(-0.697)	(-0.599)	(-0.630)	(-0.633)	
O6	-0.769	-0.742	-0.756	-0.732	-0.636	-0.736	-0.728	-0.718	-0.711	-0.648
	(-0.870)	(-0.828)	(-0.837)	(-0.815)		(-0.860)	(-0.595)	(-0.795)	(-0.814)	
O38	-0.769	-0.742	-0.726	-0.733	-0.636	-0.736	-0.728	-0.714	-0.711	-0.648
	(-0.870)	(-0.828)	(-0.779)	(-0.815)		(-0.860)	(-0.595)	(-0.827)	(-0.814)	
O21	-0.978	-0.952	-0.960	-0.930	-0.963	-0.987	-0.964	-0.957	-0.940	-0.921
	(-0.970)	(-0.941)	(-0.980)	(-0.923)		(-0.978)	(-0.527)	(-0.973)	(-0.931)	
μ	2.335	2.730	1.594	2.428	0.263	1.919	3.842	2.614	3.150	1.699
	(2.001)	(4.116)	(3.530)	(0.844)		(8.648)	(9.962)	(5.948)	(5.621)	

***The value in parentheses indicates the zwitterionic complex.**

$ Data not available