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Interactions of di-Imine Copper(II) Complexes with Albumin: Competitive Equilibria, Promoted Oxidative Damage and DFT Studies

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Table S1. Bond critical point properties (a.u.) of complexes [CuL] **1-6** and $[Cu(BSA)]^+$ at the BP86/TZVP level

	$[Cu(apzpn)]^{2+}$						$[Cu(apzepy)(H_2O)]^{2+}$				
Bonds	ρ_b	$\nabla^2\rho_b$	G_b	V_b	H_b	Bonds	ρ_b	$\nabla^2\rho_b$	G_b	V_b	H_b
C-N	0.332	–0.878	0.499	–1.217	–0.718	C-N	0.332	–0.858	0.503	–1.220	–0.717
C-N	0.331	–0.865	0.498	–1.212	–0.714	C-N	0.319	–0.876	0.444	–1.108	–0.663
C-N	0.319	–0.878	0.444	–1.107	–0.663	C-N	0.358	–0.920	0.573	–1.376	–0.803
C-N	0.360	–0.936	0.575	–1.384	–0.809	C-N	0.256	–0.576	0.280	–0.704	–0.424
C-N	0.251	–0.548	0.263	–0.662	–0.400	C-N	0.315	–0.850	0.439	–1.090	–0.651
C-N	0.359	–0.952	0.573	–1.384	–0.811	C-N	0.317	–0.850	0.446	–1.106	–0.659
	0.325[a]	**–0.843**	**0.475**	**–1.161**	**–0.686**		**0.316**	**–0.822**	**0.448**	**–1.101**	**–0.653**
Cu-N	0.092	0.323	0.028	0.026	0.053	Cu-N	0.090	0.323	0.026	0.029	0.055
Cu-N	0.086	0.312	0.024	0.030	0.054	Cu-N	0.094	0.316	0.028	0.023	0.051
Cu-N	0.094	0.325	0.029	0.024	0.052	Cu-N	0.096	0.328	0.030	0.023	0.052
Cu-N	0.086	0.311	0.024	0.030	0.054		**0.093**	**0.322**	**0.028**	**0.025**	**0.053**
	0.090	**0.318**	**0.026**	**0.027**	**0.053**	Cu-O	**0.048**	**0.227**	**0.005**	**0.046**	**0.051**
	$[Cu(pyalen)]^{2+}$						$[Cu(dachist)]^{2+}$				
Bonds	ρ_b	$\nabla^2\rho_b$	G_b	V_b	H_b	Bonds	ρ_b	$\nabla^2\rho_b$	G_b	V_b	H_b
C-N	0.370	–0.855	0.612	–1.438	–0.826	C-N	0.250	–0.545	0.257	–0.650	–0.393
C-N	0.252	–0.556	0.268	–0.675	–0.407	C-N	0.361	–0.953	0.578	–1.394	–0.816
C-N	0.252	–0.556	0.268	–0.675	–0.407	C-N	0.361	–0.944	0.342	–0.921	–0.578
C-N	0.370	–0.858	0.612	–1.438	–0.826	C-N	0.250	–0.546	0.258	–0.652	–0.394
C-N	0.313	–0.864	0.414	–1.044	–0.630	C-N	0.297	–0.748	0.375	–0.937	–0.562
C-N	0.331	–0.894	0.491	–1.206	–0.715	C-N	0.337	–0.970	0.483	–1.210	–0.726
C-N	0.330	–0.888	0.491	–1.204	–0.713	C-N	0.337	–0.971	0.483	–1.209	–0.726
C-N	0.313	–0.864	0.414	–1.044	–0.630	C-N	0.297	–0.747	0.375	–0.937	–0.562
	0.316	**–0.792**	**0.446**	**–1.091**	**–0.644**		**0.311**	**–0.803**	**0.394**	**–0.989**	**–0.595**
Cu-N	0.096	0.336	0.030	0.024	0.054	Cu-N	0.088	0.304	0.025	0.026	0.051
Cu-N	0.096	0.335	0.030	0.024	0.054	Cu-N	0.088	0.306	0.025	0.027	0.052
Cu-N	0.084	0.300	0.023	0.029	0.052	Cu-N	0.094	0.347	0.028	0.030	0.059
Cu-N	0.084	0.300	0.023	0.029	0.052	Cu-N	0.094	0.347	0.028	0.030	0.058
	0.090	**0.318**	**0.027**	**0.026**	**0.053**		**0.091**	**0.326**	**0.027**	**0.028**	**0.055**

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Table S1. Bond critical point properties (a.u.) of complexes [CuL] **1-6** and $[Cu(BSA)]^+$ at the BP86/TZVP level (cont.)

	$[Cu(BSA)]^+$						$[Cu(apyepy)(H_2O)]^{2+}$				
Bonds	ρ_b	$\nabla^2\rho_b$	G_b	V_b	H_b	Bonds	ρ_b	$\nabla^2\rho_b$	G_b	V_b	H_b
C-N	0.247	–0.529	0.248	–0.629	–0.380	C-N	0.328	–0.867	0.485	–1.187	–0.702
C-N	0.292	–0.769	0.335	–0.862	–0.527	C-N	0.317	–0.875	0.432	–1.082	–0.650
C-N	0.241	–0.487	0.236	–0.594	–0.358	C-N	0.359	–0.917	0.578	–1.385	–0.807
C-N	0.271	–0.633	0.281	–0.720	–0.439	C-N	0.252	–0.558	0.267	–0.673	–0.406
C-N	0.240	–0.489	0.221	–0.563	–0.343	C-N	0.318	–0.860	0.450	–1.114	–0.665
C-N	0.342	–1.001	0.498	–1.247	–0.748	C-N	0.318	–0.850	0.452	–1.116	–0.664
C-N	0.294	–0.733	0.366	–0.916	–0.550		**0.315**	**–0.821**	**0.444**	**–1.093**	**–0.649**
	0.275	**–0.663**	**0.312**	**–0.790**	**–0.478**	Cu-N	0.095	0.343	0.029	0.028	0.057
Cu-N	0.043	–0.033	0.134	0.005	0.024	Cu-N	0.094	0.319	0.028	0.023	0.051
Cu-N	0.073	–0.058	0.232	0.018	0.022	Cu-N	0.098	0.343	0.031	0.023	0.055
Cu-N	0.075	–0.063	0.251	0.018	0.027		**0.096**	**0.335**	**0.030**	**0.025**	**0.054**
Cu-N	0.102	–0.097	0.387	0.033	0.031	Cu-O	**0.059**	**0.277**	**0.010**	**0.049**	**0.059**
	0.064	**–0.051**	**0.206**	**0.013**	**0.024**						

	$[Cu(apzhist)(H_2O)]^{2+}$				
Bonds	ρ_b	$\nabla^2\rho_b$	G_b	V_b	H_b
C-N	0.336	–0.962	0.238	–0.717	–0.479
C-N	0.296	–0.739	0.192	–0.569	–0.377
C-N	0.327	–0.848	0.271	–0.753	–0.483
C-N	0.297	–0.678	0.245	–0.660	–0.415
C-N	0.252	–0.556	0.132	–0.404	–0.271
C-N	0.359	–0.923	0.343	–0.917	–0.574
	0.311	**–0.784**	**0.237**	**–0.670**	**–0.433**
Cu-N	0.102	0.371	0.125	–0.158	–0.033
Cu-N	0.087	0.285	0.096	–0.121	–0.025
Cu-N	0.092	0.332	0.111	–0.138	–0.028
	0.094	**0.329**	**0.111**	**–0.139**	**–0.029**
Cu-O	**0.049**	**0.229**	**0.063**	**–0.069**	**–0.006**

[a] Average values are depicted in bold type.