Supporting Materials

A New Zn(II) Azido Complex of L-Arginine: X-ray Crystal Structure, Hirshfeld, and AIM Studies

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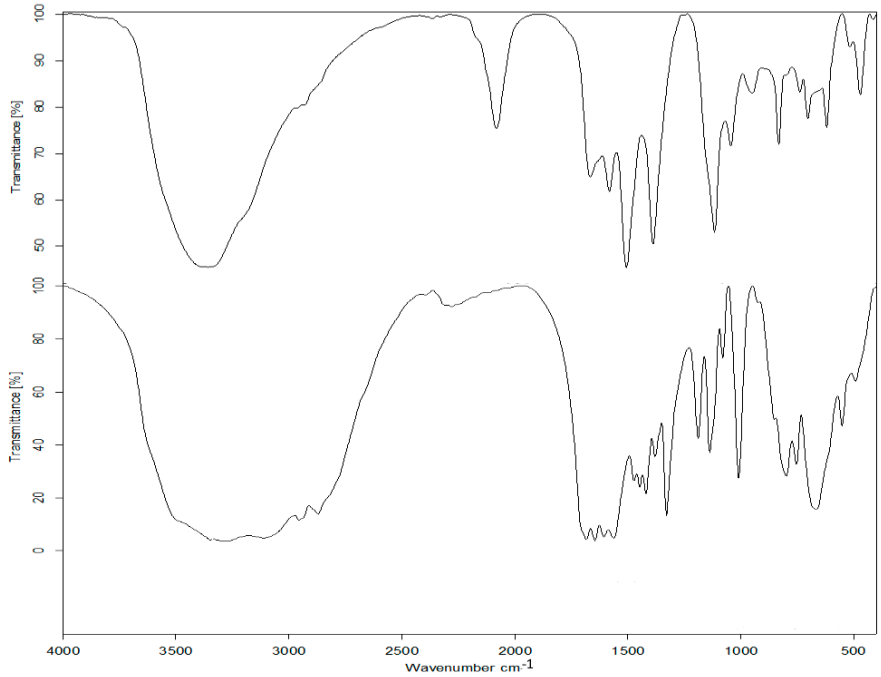

Figure S1. FTIR spectra of the $[Zn(N_3)(Arg)_2](N_3)\cdot 3H_2O$ complex; (upper) and the free ligand (Arg); (lower).

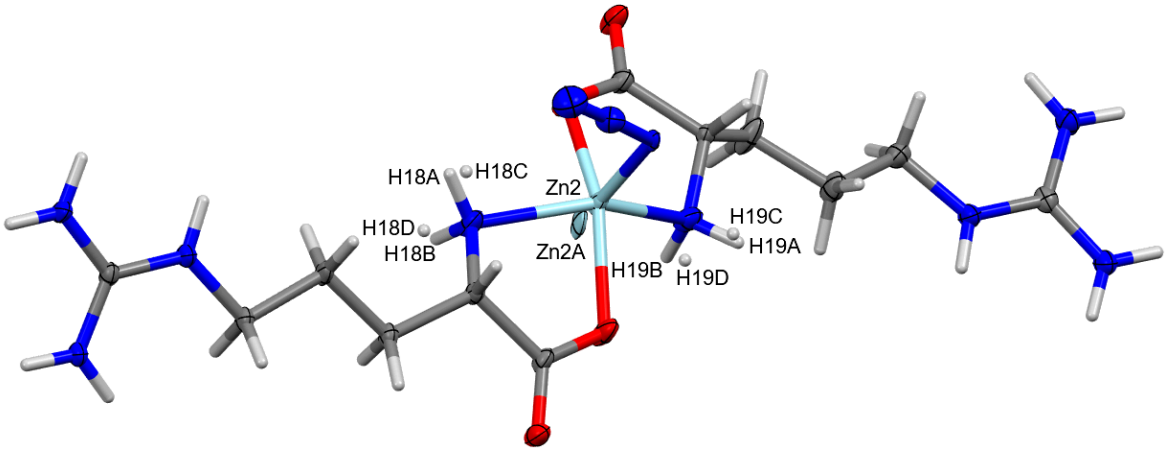

Figure S2. The disorder of the $[Zn(N_3)(Arg)_2](N_3)\cdot 3H_2O$ complex for molecule **B** (major 94% and minor 6%).

Table S1. The topological parameters (a.u.) at the Zn–N, Zn–O and N-N bond critical points (BCPs) using WB97XD method and the cc-pVTZ basis set.

Bond	ρ(r)	G(r)	V(r)	H(r)	$\nabla^2\rho(r)$	|V(r)|/G(r)
Zn1-N1	0.0603	0.0843	-0.0955	-0.0112	0.2923	1.1329
Zn1-N4	0.0684	0.0700	-0.0883	-0.0183	0.2069	1.2614
Zn1-N5	0.0711	0.0761	-0.0955	-0.0194	0.2269	1.2550
Zn1-O1	0.0750	0.0757	-0.1000	-0.0243	0.2054	1.3210
Zn1-O3	0.0786	0.0809	-0.1063	-0.0254	0.2218	1.3140
Zn2-N15	0.0803	0.1238	-0.1441	-0.0202	0.4144	1.1640
Zn2-N19	0.0703	0.0679	-0.0853	-0.0173	0.2025	1.2563
Zn2-N18	0.0707	0.0716	-0.0880	-0.0163	0.2213	1.2291
Zn2-O7	0.0717	0.0748	-0.0934	-0.0186	0.2250	1.2487
Zn2-O5	0.0733	0.0775	-0.0971	-0.0196	0.2317	1.2529
N1-N2	0.5852	0.5463	-1.6396	-1.0933	-2.1879	3.0013
N2-N3	0.4852	0.4756	-1.2525	-0.7769	-1.2050	2.6333
N15-N16	0.4668	0.4075	-1.1184	-0.7109	-1.2134	2.7443
N16-N17	0.5279	0.5093	-1.4064	-0.8971	-1.5508	2.7612
N12-N13	0.5196	0.5297	-1.4395	-0.9098	-1.5204	2.7176
N13-N14	0.5134	0.4792	-1.3680	-0.8889	-1.6387	2.8550
N26-N27	0.5290	0.5198	-1.4291	-0.9092	-1.5575	2.7490
N27-N28	0.5056	0.4004	-1.1994	-0.7991	-1.5948	2.9958