Supplementary Information

AdcA lipoprotein involved in Zn(II) transport in *Streptococcus mutans* – is it as metal-specific as expected?

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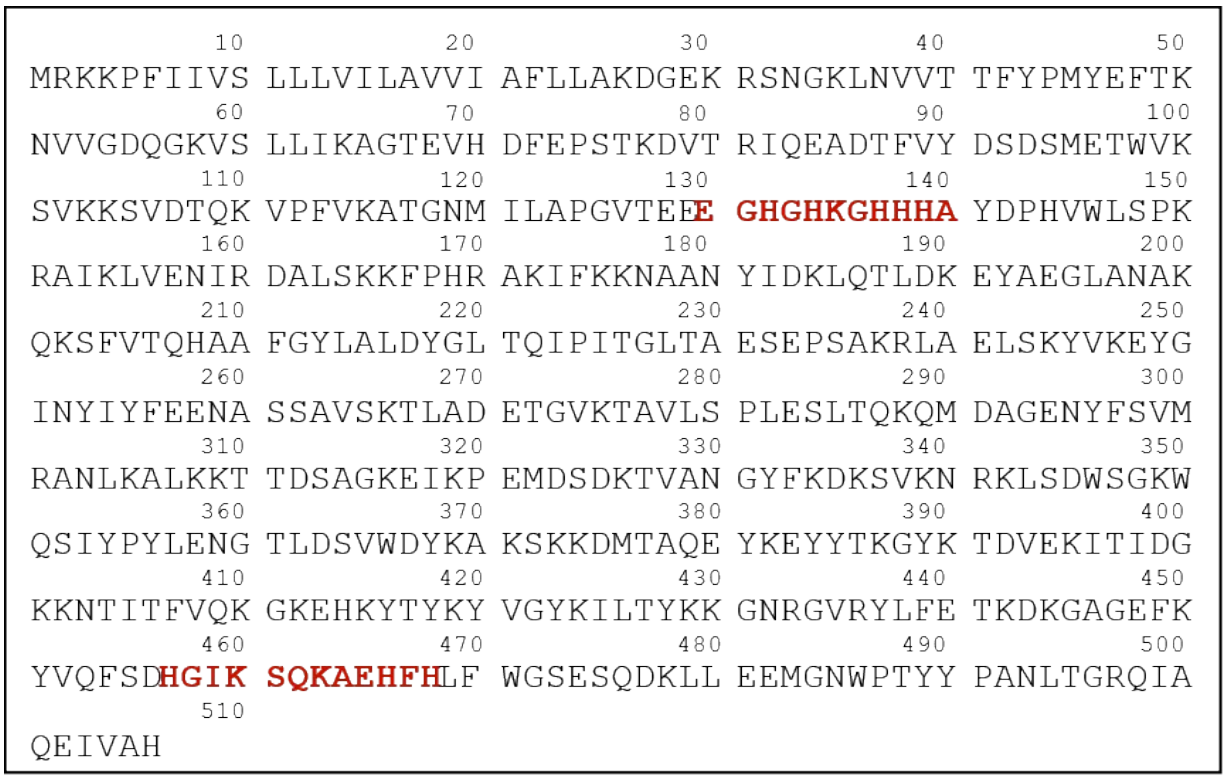
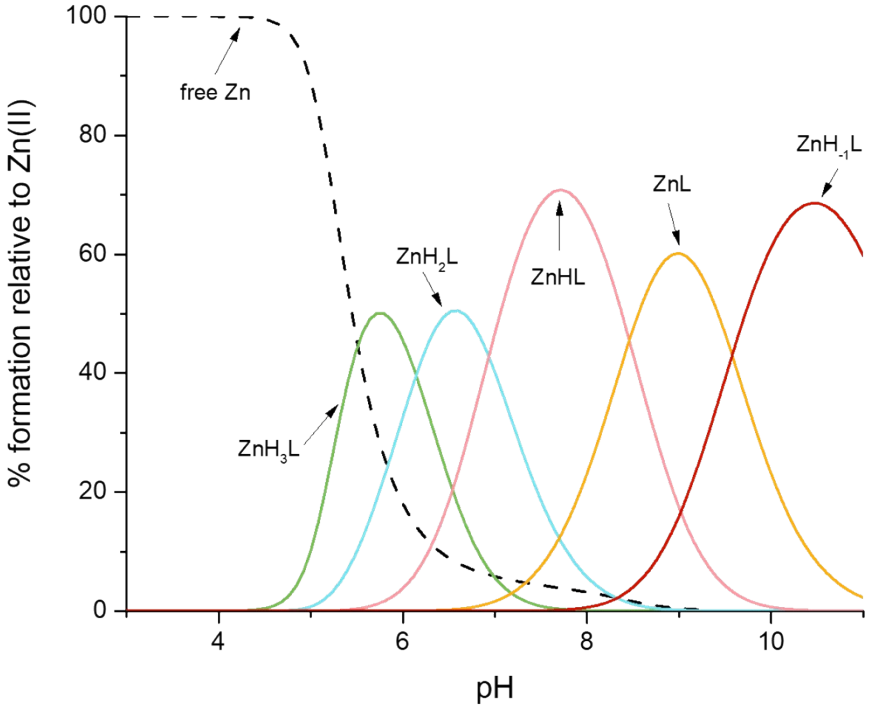


Figure 1. Amino acid sequence of AdcA protein from *Streptococcus mutans*, probable Zn(II) binding sites are highlighted in red

A)



B)

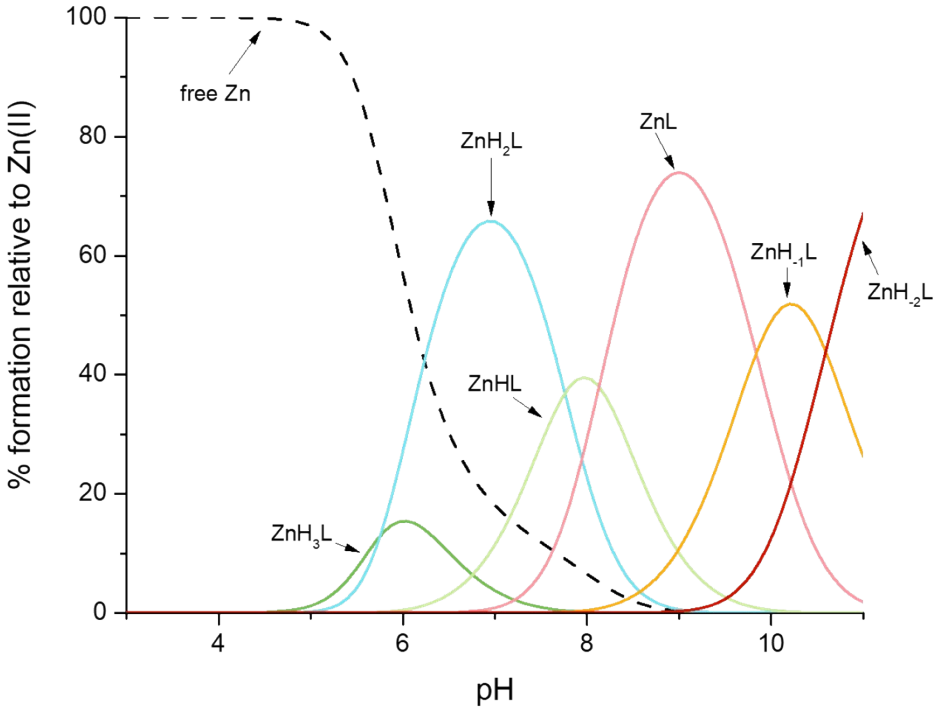
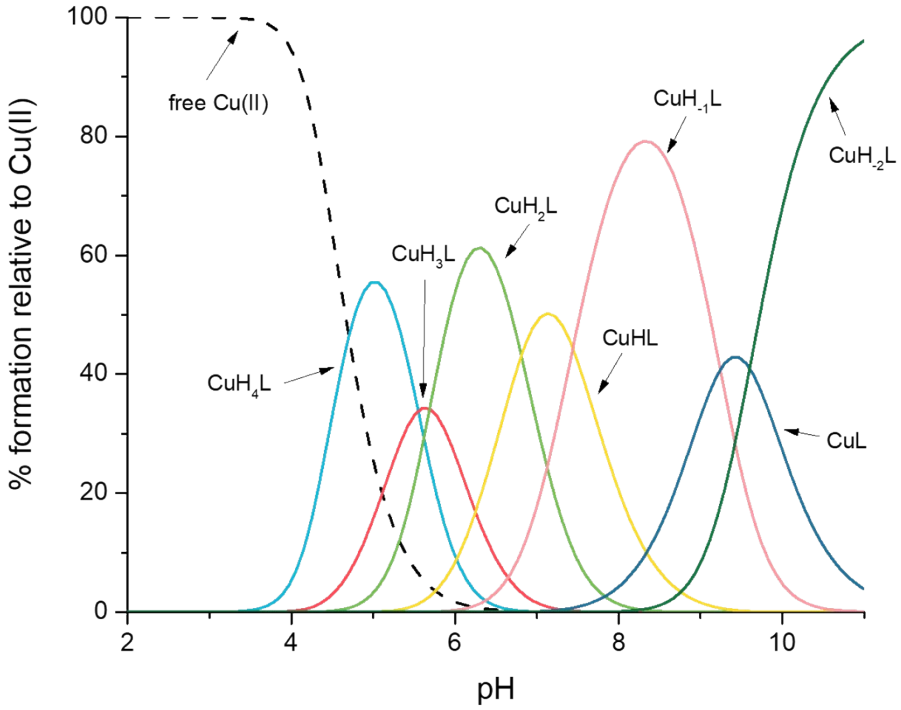


Figure 2. Species distribution diagrams for the formation of A) Zn(II) complexes with the Ac-EGHGHKGHHHA-NH_2; B) Zn(II) complexes with the Ac-HGIKSQKAEHFH-NH_2; T = 298 K; I = 0.1 M; [L] = 0.0005 M; M(II)/L molar ratio = 0.8 : 1

A)



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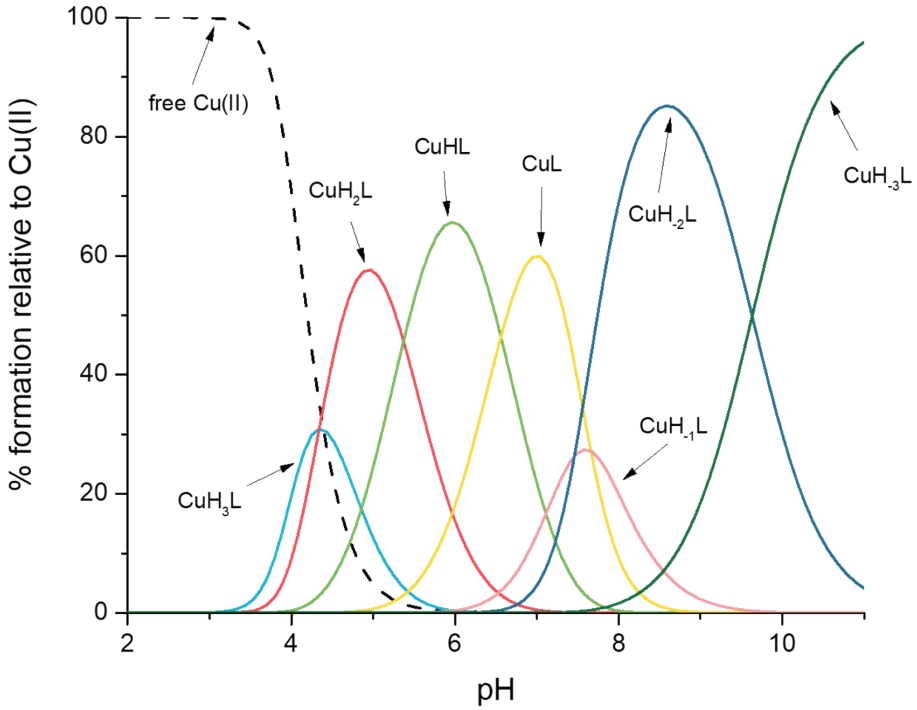

Figure 3. Species distribution diagrams for the formation of A) Cu(II) complexes with the Ac-EGHGHKGHHHA-NH_2; B) Cu(II) complexes with the Ac-HGIKSQKAEHFH-NH_2; T = 298 K; I = 0.1 M; [L] = 0.0005 M; M(II)/L molar ratio = 0.8 : 1

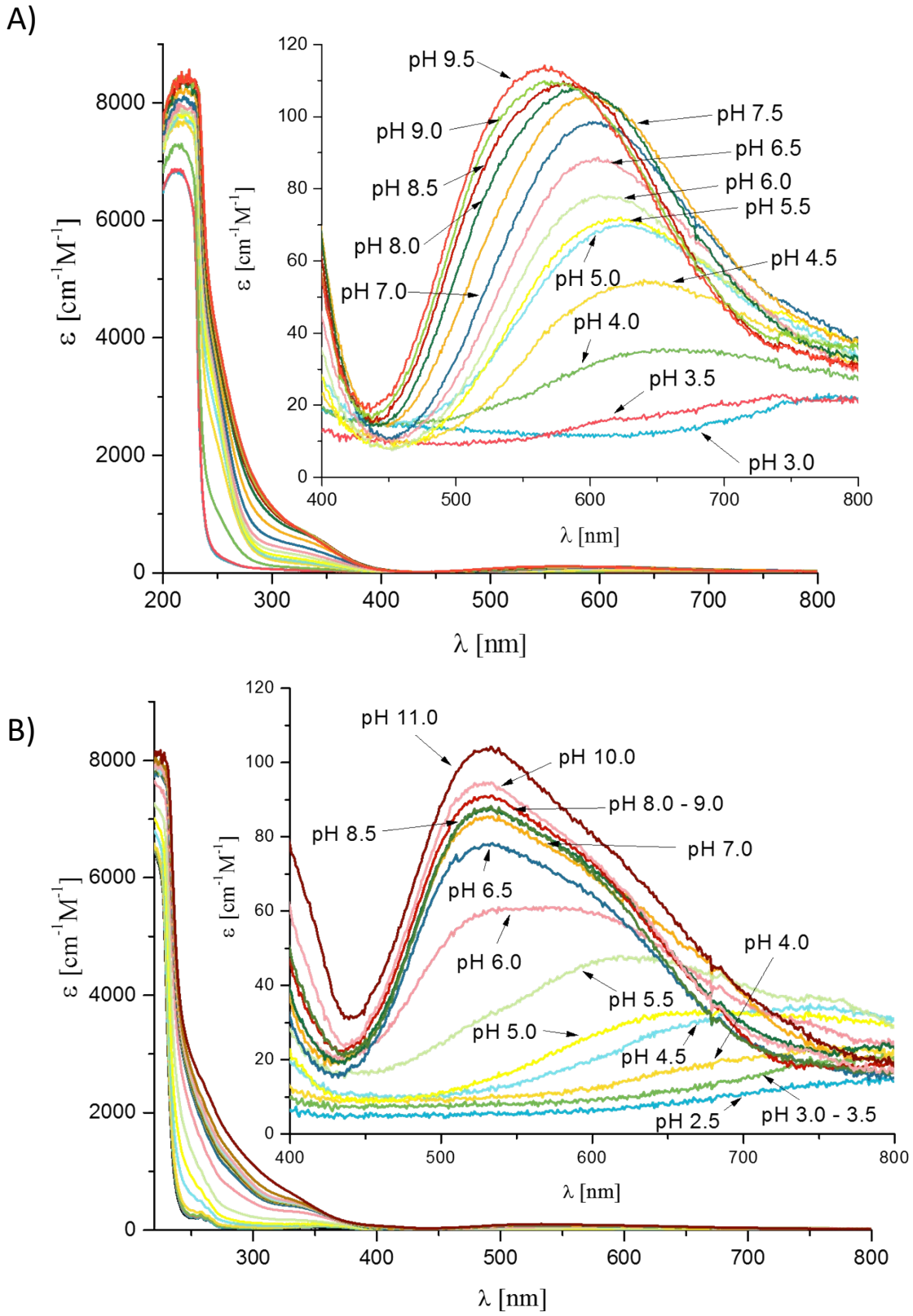

Figure 4. UV-Vis spectra of Cu(II) complexes with A) the Ac-EGHGHKGHHHA-NH_2; B) the Ac-HGIKSQKAEHFH-NH_2 in the range 200-800 nm and pH range 2.0-11.0; T = 298 K; optical path = 1 cm; [L] = 0.0005 M; M(II)/L = 0.8 : 1

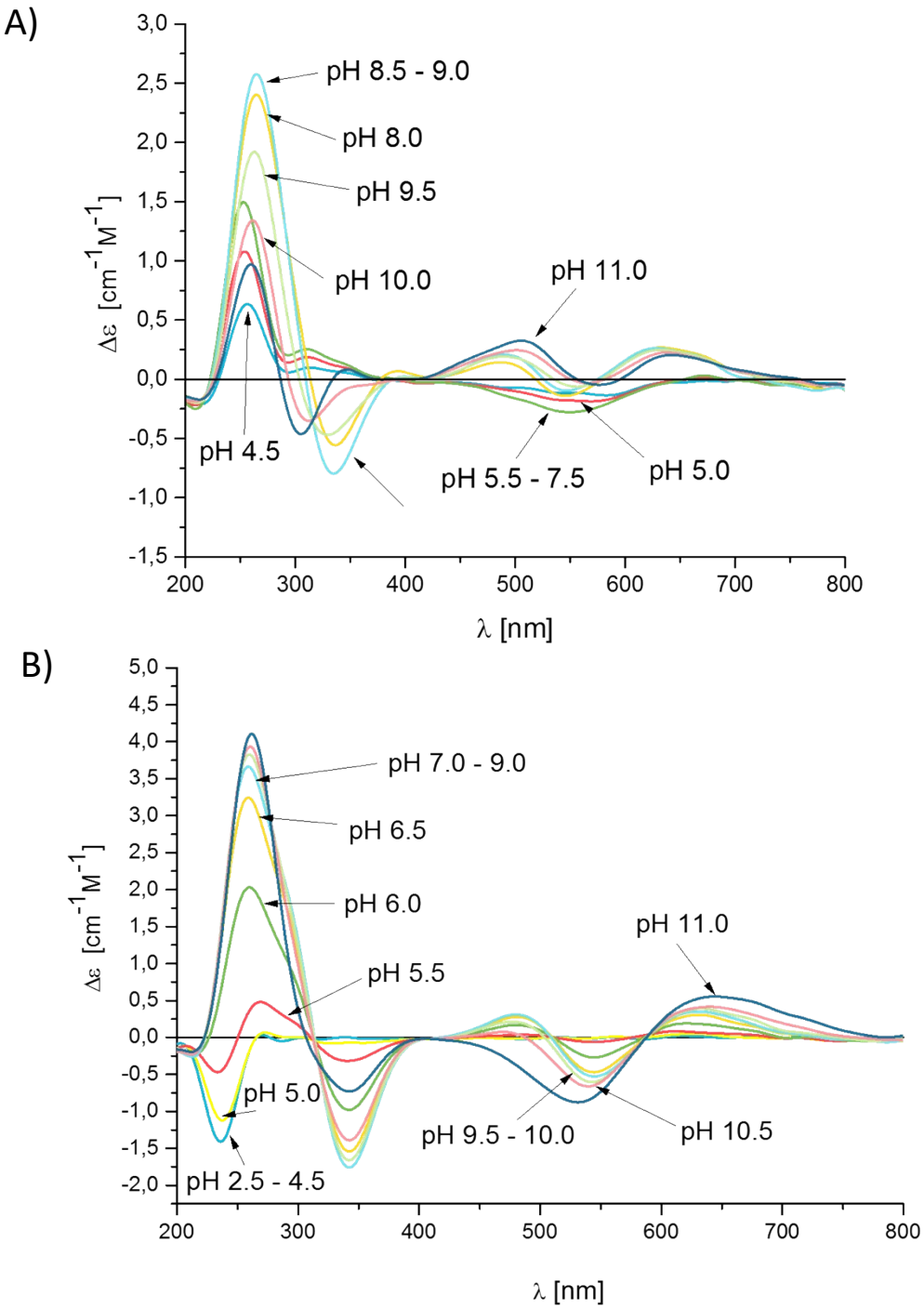

Figure 5. CD spectra of Cu(II) complexes with A) the Ac-EGHGHKGHHHA-NH_2; B) the Ac-HGIKSQKAEHFH-NH_2 in the range 200-800 nm and pH range 2.0-11.0; T = 298 K; optical path = 1 cm; [L] = 0.0005 M; M(II)/L = 0.8 : 1

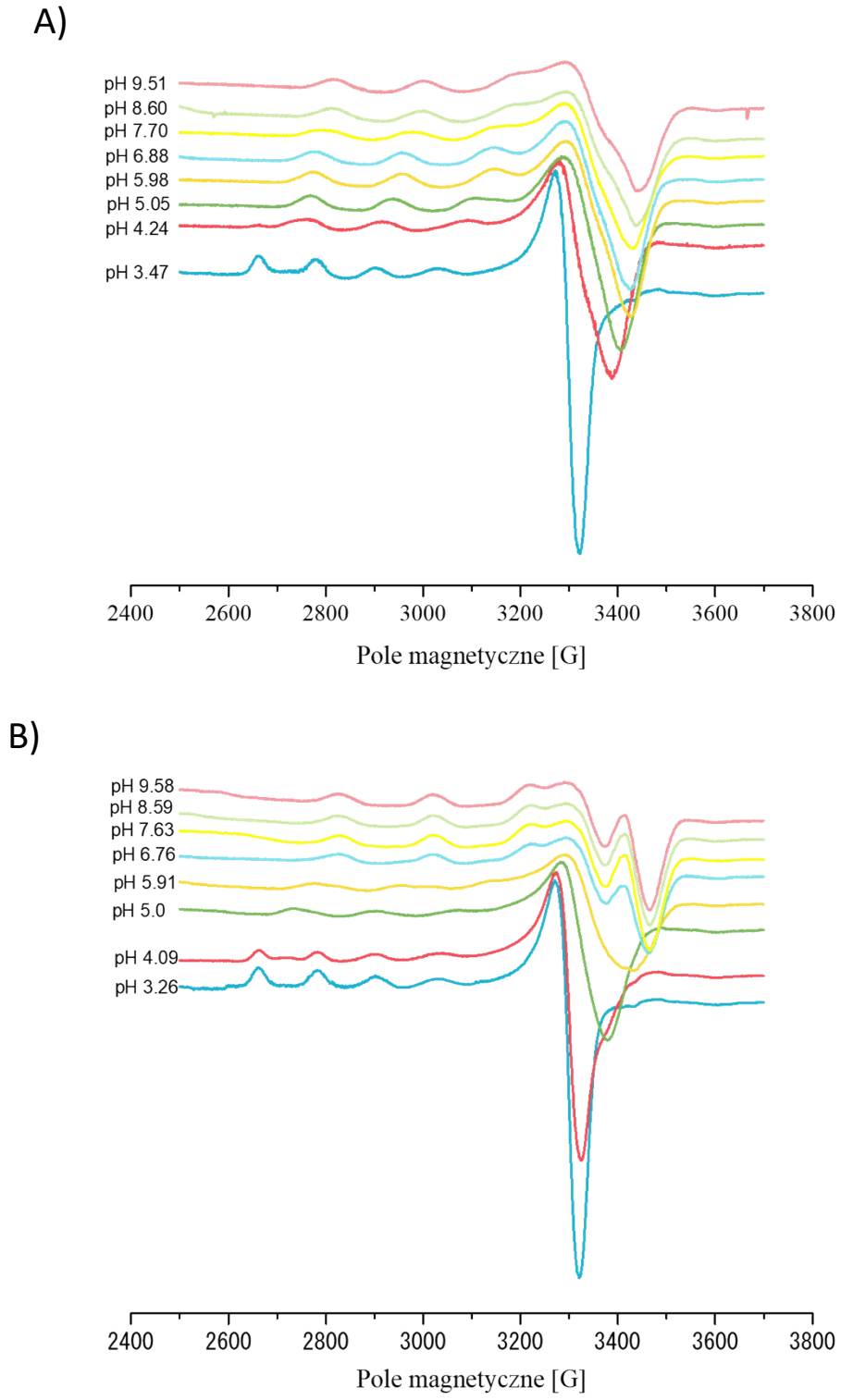

Figure 6. EPR spectra of Cu(II) complexes with A) the Ac-EGHGHKGHHHA-NH_2; B) the Ac-HGIKSQKAEHFH-NH_2

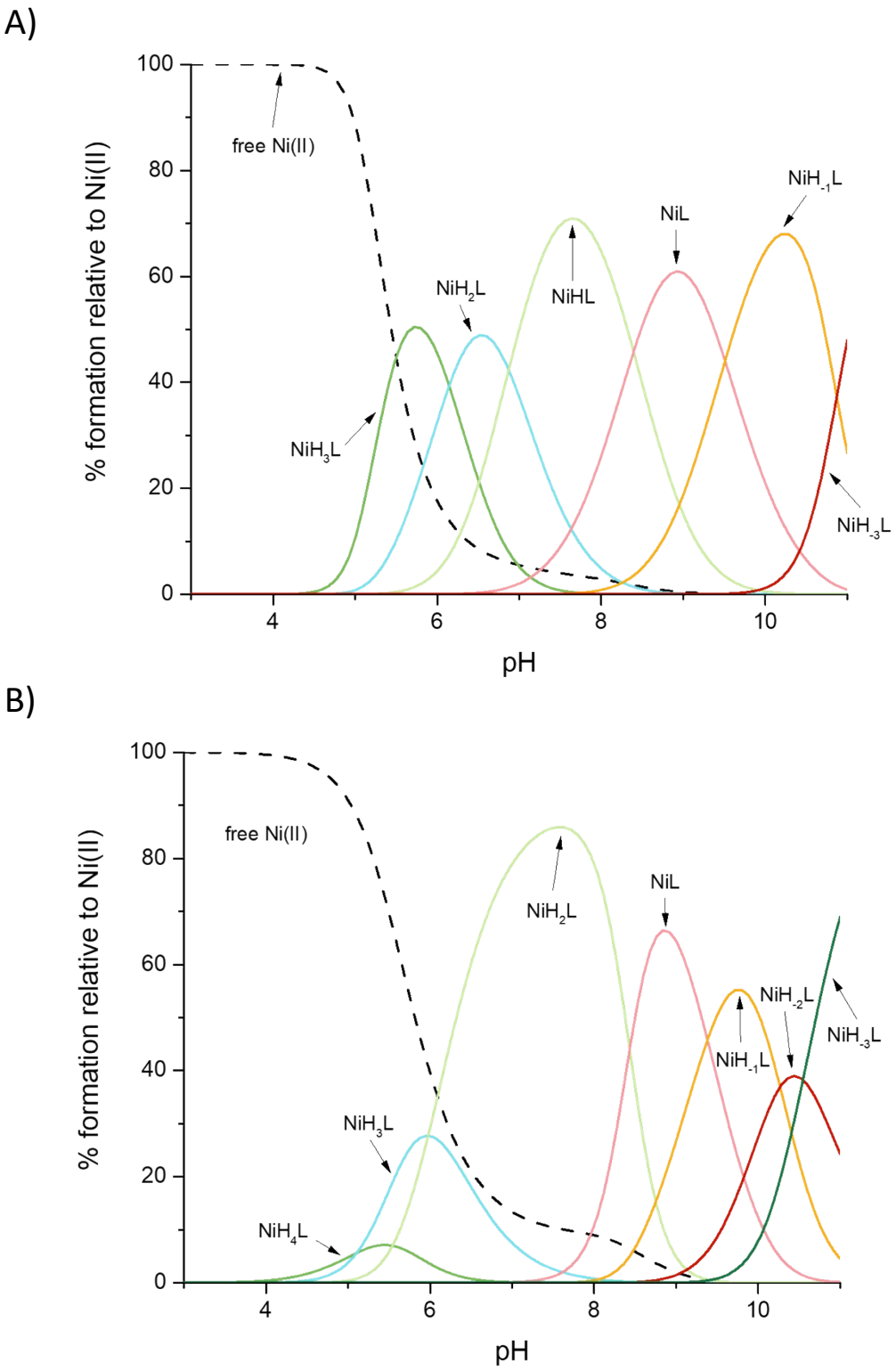

Figure 7. Species distribution diagrams for the formation of A) Ni(II) complexes with the Ac-EGHGHKGHHHA-NH_2; B) Ni(II) complexes with the Ac-HGIKSQKAEHFH-NH_2 ; T = 298 K; I = 0.1 M; [L] = 0.0005 M; M(II)/L molar ratio = 0.8 : 1

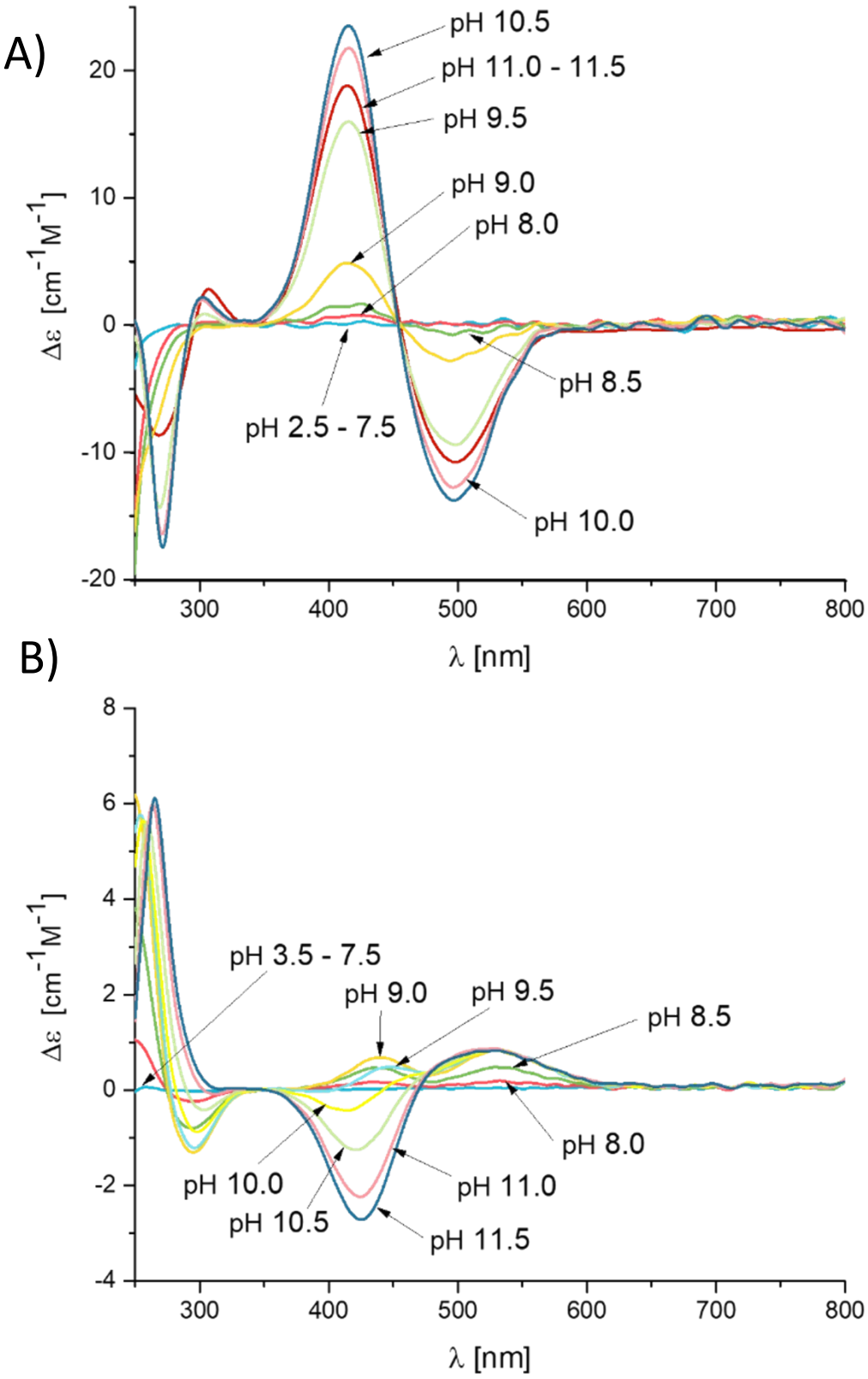

Figure 8. CD spectra of Ni(II) complexes with A) the Ac-EGHGHKGHHHA-NH_2; B) the Ac-HGIKSQKAEHFH-NH_2 in the range 250-800 nm and pH range 2.5-10.5; T = 298 K; optical path = 1 cm; [L] = 0.0005 M; M(II)/L = 0.8 : 1

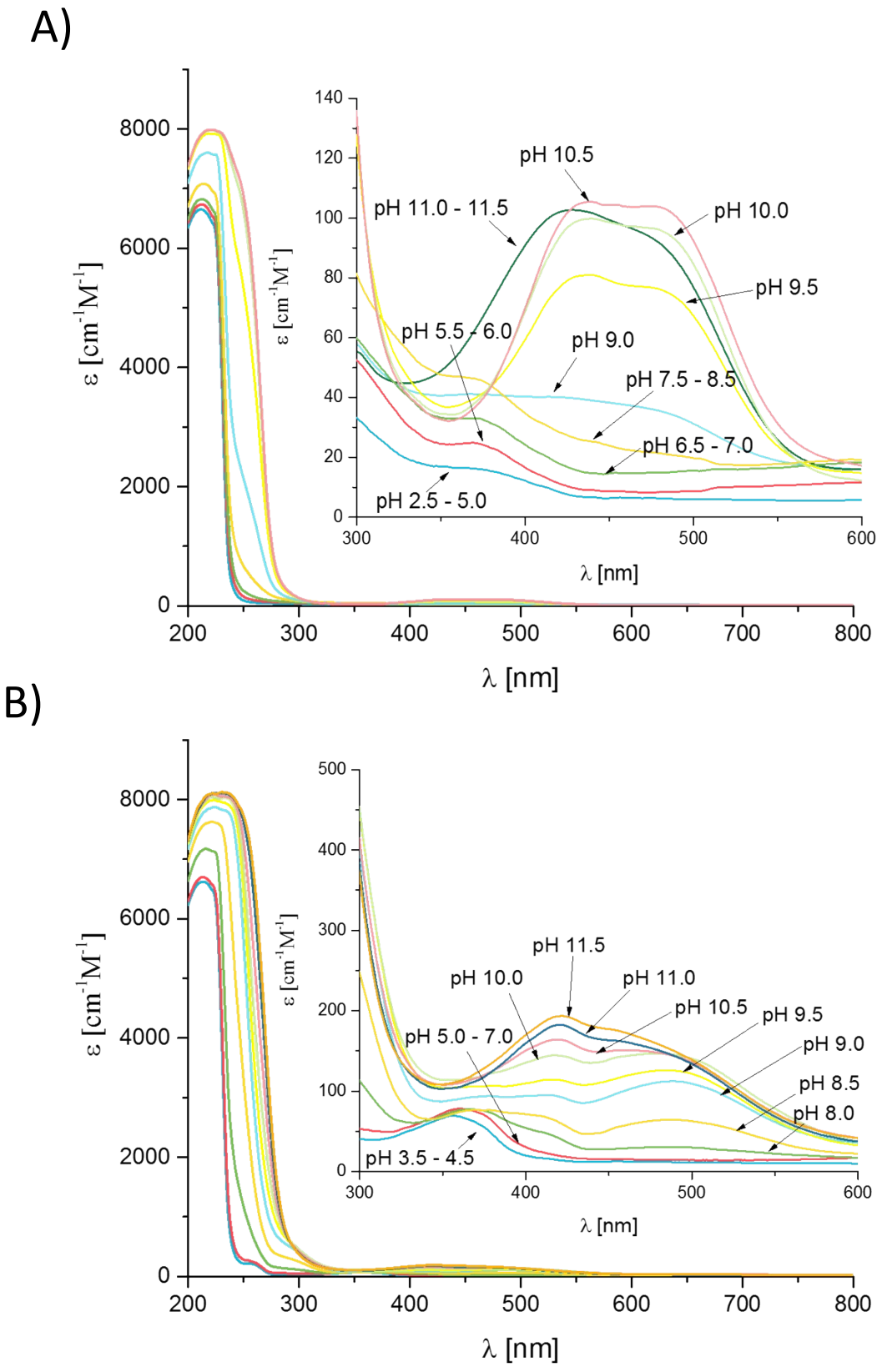

Figure 9. UV-Vis spectra of Ni(II) complexes with A) the Ac-EGHGHKGHHHA-NH_2; B) the Ac-HGIKSQKAEHFH-NH_2 in the range 200-800 nm and pH range 2.5-10.5; T = 298 K; optical path = 1 cm; [L] = 0.0005 M; M(II)/L = 0.8 : 1

Table 1 Equilibrium constants for Ac-EGHGHKGHHHA-NH_2 ligand, spectroscopic parameters and proposed coordination modes for Cu(II) complexes at T = 298 K and I = 0.1 M ($NaClO_4$); M(II)/L = 0.8 : 1

Ac-EGHGHKGHHHA-NH_2									
	Log β	**Log*K***	**UV-Vis**		**CD**		**EPR**		
			λ ***[nm]***	***ε*** ***[M^{-1}·cm^{-1}]***	***λ*** ***[nm]***	***Δε*** ***[M^{-1}·cm^{-1}]***	***A_{II}*** ***[G]***	***g_{II}***	
CuH_4L	36.62 (1)		328 640	154.16 54.81	256 314 540	0.64 0.10 -0.11	150	2.31	**$1N_{im}$ /$2N_{im}$**
CuH_3L	32.28 (1)	4.34	328 627	188.17 69.96	254 311 554	1.08 0.19 -0.18	171	2.28	**$2N_{im}$**
CuH_2L	26.91 (2)	5.37	334 606	271.39 78.29	253 308 546	1.65 0.29 -0.30	188	2.25	**$3N_{im}$**
CuHL	20.35 (2)	6.56	331 604	433.12 98.51	256 385 545 643	1.53 0.04 -0.22 0.11	188	2.25	**$2N_{im}1N^-$**
CuL	12.69 (3)	7.66	333 593	637.11 108.24	264 334 392 488 546 634	2.40 -0.55 0.07 0.14 -0.14 0.27	195	2.23	**$1N_{im}2N^-$**
$CuH_{-1}L$	5.23 (3)	7.46	331 571	699.61 109.82	265 335 488 547 634	2.60 -0.76 0.20 -0.14 0.26	205	2.21	**$1N_{im}3N^-$**
$CuH_{-2}L$	-4.40 (5)	9.63	337 562	611.55 113.24	263 329 490 556 633	1.92 -0.47 0.19 -0.06 0.25	205	2.21	**$1N_{im}3N^-$**

Table 2 Equilibrium constants for Ac-HGIKSQKAEHFH-NH_2 ligand, spectroscopic parameters and proposed coordination modes for Cu(II) complexes at T = 298 K and I = 0.1 M ($NaClO_4$); M(II)/L = 0.8 : 1

Ac-HGIKSQKAEHFH-NH_2									
	Log*β*	**Log*K***	**UV-Vis**		**CD**		**EPR**		**Binding mode**
			λ ***[nm]***	***ε*** ***[$M^{-1}\cdot cm^{-1}$]***	***λ*** ***[nm]***	***Δε*** ***[$M^{-1}\cdot cm^{-1}$]***	***A_{II}*** ***[G]***	***g_{II}***	
CuH_3L	33.73 (3)		352 672	104.99 32.28	238	-2.19	152	2.31	**$1N_{im}/2N_{im}$**
CuH_2L	28.18 (5)	5.55	346 619	156.69 47.99	233 269 341	-0.47 0.48 -0.32	170	2.26	**$3N_{im}$**
CuHL	22.49 (4)	5.69	336 534	398.07 78.32	259 342 480 544 635	3.24 -1.54 0.32 -0.51 0.33	193	2.20	**$3N_{im}1N^-$**
CuL	15.68 (5)	6.81	335 526	430.07 85.17	259 342 481 544 630	3.57 -1.71 0.29 -0.54 0.33	195	2.20	**$2N_{im}2N^-$**
$CuH_{-1}L$	8.24 (4)	7.44	331 528	452.75 87.72	259 342 479 545 633	3.71 -1.80 0.32 -0.55 0.35	206	2.20	**$1N_{im}3N^-$**
$CuH_{-2}L$	-1.00 (7)	9.24	327 528	476.53 91.57	259 342 479 544 635	3.79 -1.77 0.29 -0.56 0.35	206	2.20	**$1N_{im}3N^-$**
$CuH_{-3}L$	-10.60 (5)	9.60	337 528	552.11 103.49	262 342 531 644	4.11 -0.73 -0.88 0.55	206	2.20	**$1N_{im}3N^-$**