Supplementary Material (ESI) for Dalton Transactions

Supplementary Information

To

Theoretical Studies on the First Proton Macroaffinity of Ni(II), Cu(II), Zn(II) and Cd(II) Complexes of four Triazacycloalkanes ([X] ane N_3, X = 9 – 12) : Good Correlations with the Formation Constants in Solution

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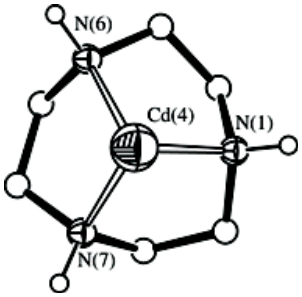

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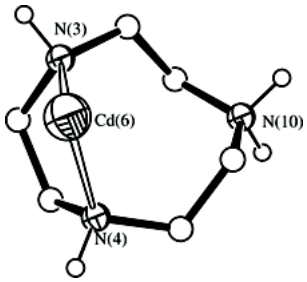

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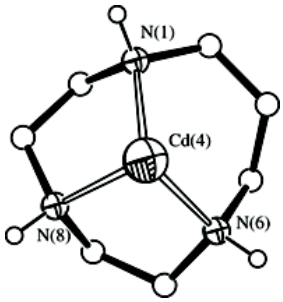

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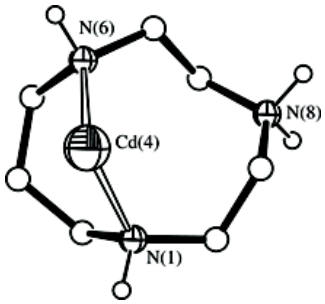

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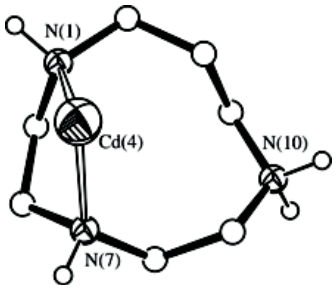

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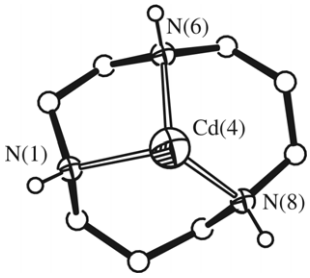

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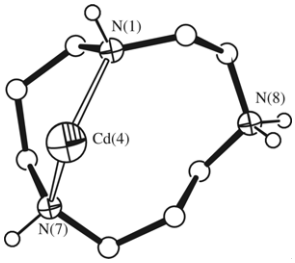

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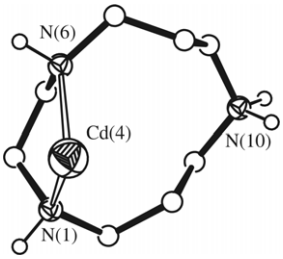

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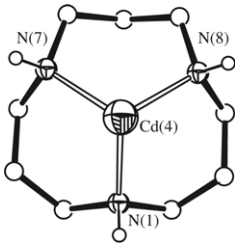

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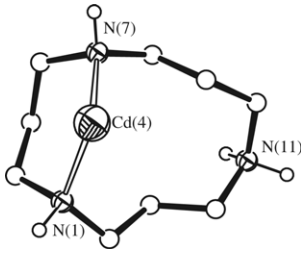

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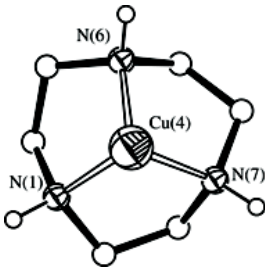
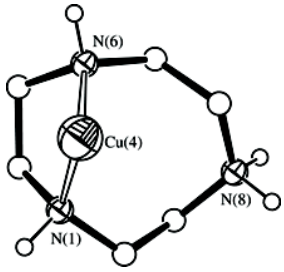
Fig. S1: The optimized structures for all $[CdL]^{2+}$ complexes and their protonated forms, $[CdHL]^{3+}$, at B3lyp level of theory





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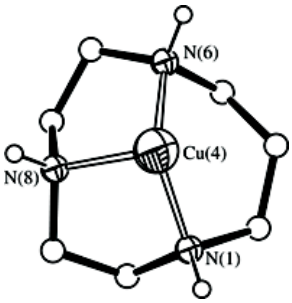

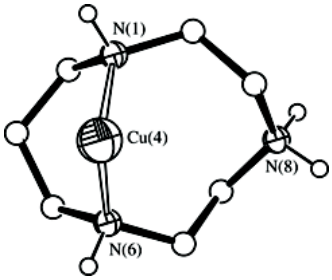

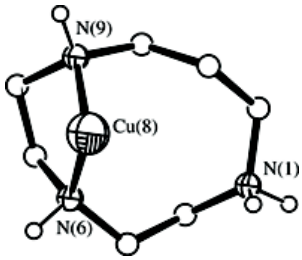

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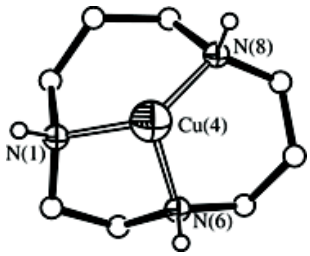

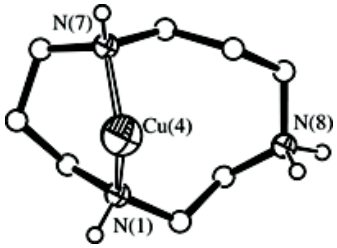

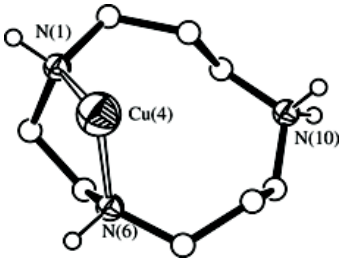

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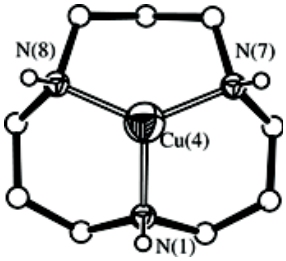

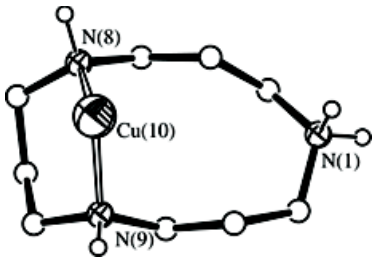

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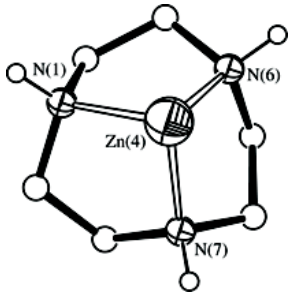
Fig. S2: The optimized structures for all $[CuL]^{2+}$ complexes and their protonated forms, $[CuHL]^{3+}$, at B3lyp level of theory



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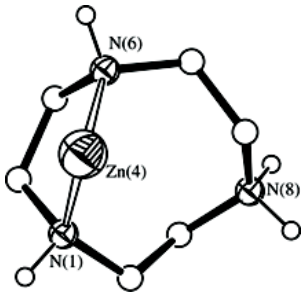

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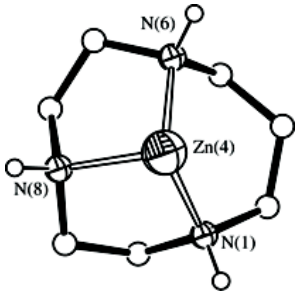

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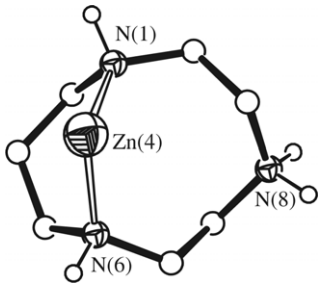

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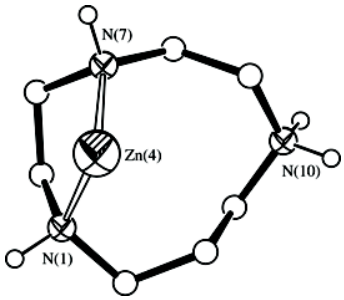

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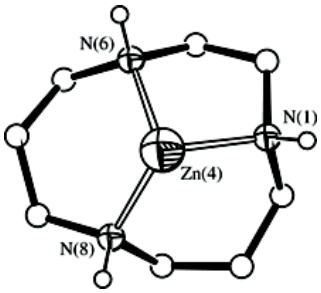

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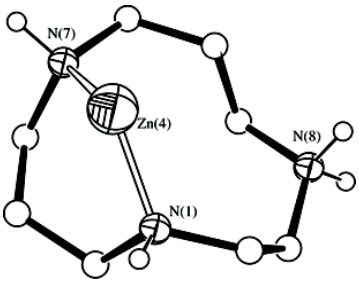

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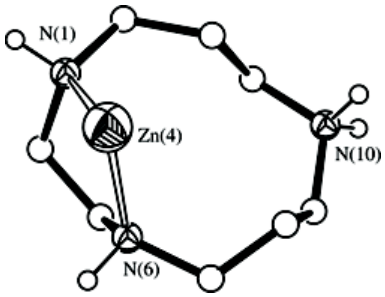

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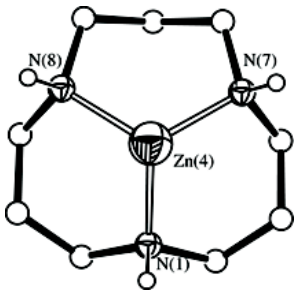

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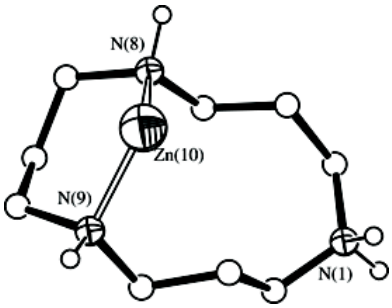

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Fig. S3: The optimized structures for all $[ZnL]^{2+}$ complexes and their protonated forms, $[ZnHL]^{3+}$, at B3lyp level of theory

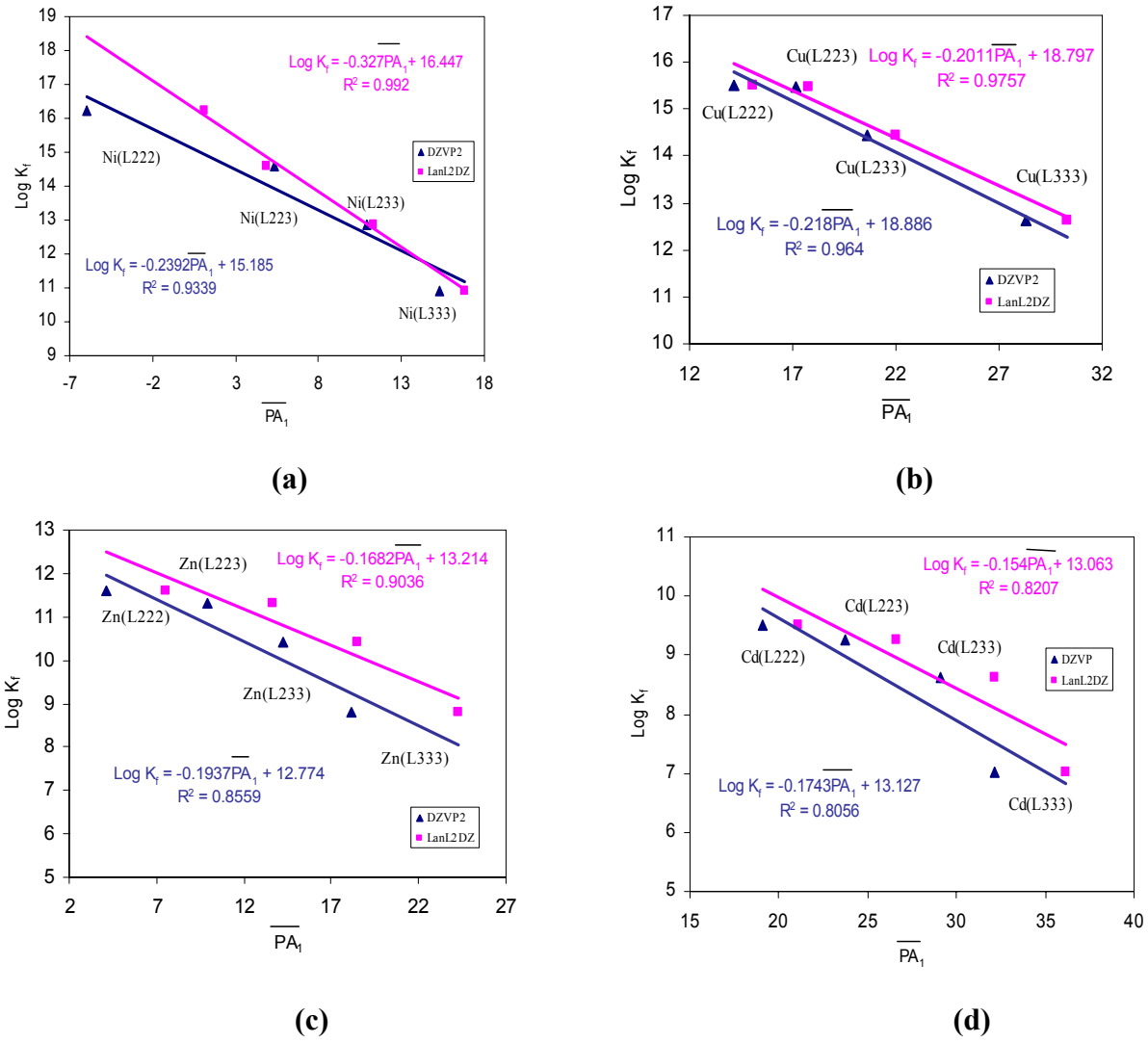


Fig. S4: Correlation of *Log* K_f vs. calculated $\overline{PA_1}$ for the first protonation step of $[NiL]^{2+}$, $[CuL]^{2+}$ $[ZnL]^{2+}$ and $[CdL]^{2+}$complexes, a, b, c and d, respectively, at B3LYP level of theory . The data are derived from Eq (2)

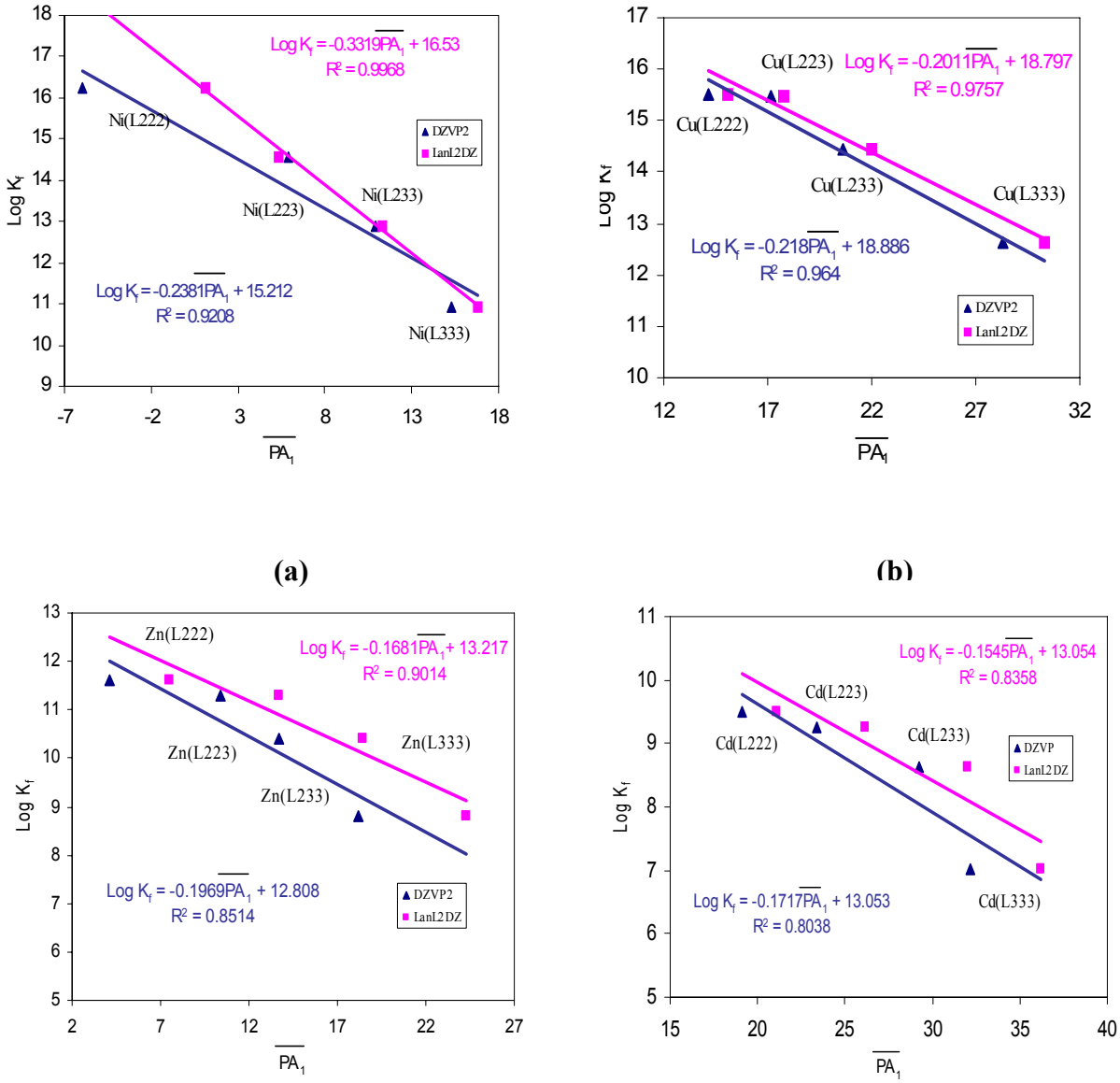


Fig. S5: Correlation of *Log* K_f vs. calculated $\overline{PA_1}$ for the first protonation step of $[NiL]^{2+}$, $[CuL]^{2+}$ $[ZnL]^{2+}$ and $[CdL]^{2+}$complexes, a, b, c and d, respectively, at B3LYP level of theory . The data are derived from Eq (3)

Table S1:
Calculated total energies (Hartree, ZPE + E_{el}), zero point energies and E_{el} of the $[ML]^{2+}$ complexes and their possible protonated forms at B3LYP level of theory with DZVP2(DZVP for Cd^{2+})basis set[a]

No.		Protonated site[b]	*ZPE*	E_0	E_{el}
I	$Ni(L222)^{2+}$		0.229837 (0.230663)	-1909.303586 (-570.382982)	-1909.533423 (-570.613645)
II	$Ni(L222H)^{3+}$	2,2	0.241697 (0.242304)	-1909.294058 (-570.384772)	-1909.535755 (-570.627076)
III	$Ni(L223)^{2+}$		0.258594 (0.259330)	-1948.617254 (-609.679196)	-1948.875848 (-609.938526)
IV	$Ni(L223H)^{3+}$	2, 2	0.269294 (0.270209)	-1948.627746 (-609.688881)	-1948.897040 (-609.959090)
V	$Ni(L223H)^{3+}$	2, 3	0.269779 (0.270581)	-1648.624680 (-609.685975)	-1948.894459 (-609.956556)
VI	$Ni(L233)^{2+}$		0.286855 (0.287663)	-1987.925013 (-648.969471)	-1988.211868 (-649.257134)
VII	$Ni(L233H)^{3+}$	2, 3	0.298143 (0.298890)	-1987.942575 (-648.987528)	-1988.240718 (-649.286418)
VIII	$Ni(L233H)^{3+}$	3, 3	0.298913 (0.299895)	-1987.942057 (-648.987602)	-1988.240970 (-649.287497)
IX	$Ni (L333)^{2+}$		0.315850 (0.316704)	-2027.232676 (-688.259096)	-2027.548526 (-688.575800)
X	$Ni(L333H)^{3+}$	3,3	0.326977 (0.328326)	-2027.257052 (-688.285842)	-2027.584029 (-688.614168)
I	$Cu(L222)^{2+}$		0.227910 (0.228787)	-2041.417219 (-597.189122)	-2041.645129 (-597.417909)
II	$Cu(L222H)^{3+}$	2,2	0.240713 (0.241213)	-2041.439748 (-597.213157)	-2041.680461 (-597.454370)
III	$Cu (L223)^{2+}$		0.257038 (0.257880)	-2080.732488 (-636.487734)	-2080.989526 (-636.745614)
IV	$Cu(L223H)^{3+}$	2, 2	0.268958 (0.269558)	-2080.762645 (-636.518514)	-2081.031603 (-636.788072)
V	$Cu(L223H)^{3+}$	2, 3	0.268856 (0.269688)	-2080.758342 (-636.514798)	-2081.027198 (-636.784486)
VI	$Cu (L233)^{2+}$		0.285495 (0.286313)	-2120.045359 (-675.782761)	-2120.330854 (-676.069074)
VII	$Cu(L233H)^{3+}$	2, 3	0.297366 (0.298187)	-2120.078399 (-675.817674)	-2120.375765 (-676.115861)
VIII	$Cu(L233H)^{3+}$	3, 3	0.298513 (0.299198)	-2120.077801 (-675.817984)	-2120.376314 (-676.117182)
IX	$Cu (L333)^{2+}$		0.314182 (0.315116)	-2159.357220 (-715.077320)	-2159.671402 (-715.392436)
X	$Cu(L333H)^{3+}$	3,3	0.327129 (0.328025)	-2159.402285 (-715.125612)	-2159.729414 (-715.453677)
I	$Zn(L222)^{2+}$		0.229797 (0.230589)	-2180.326328 (-466.678514)	-2180.556125 (-466.909103)
II	$Zn(L222H)^{3+}$	2,2	0.241773 (0.242765)	-2180.332952 (-466.690546)	-2180.574725 (-466.933311)
III	$Zn(L223)^{2+}$		0.258216 (0.259058)	-2219.638337 (-505.971009)	-2219.896553 (-506.230067)
IV	$Zn(L223H)^{3+}$	2, 2	0.269907 (0.270862)	-2219.656312 (-505.993006)	-2219.926219 (-506.263868)
V	$Zn(L223H)^{3+}$	2, 3	0.270240 (0.271464)	-2219.652985 (-505.992667)	-2219.923225 (-506.264131)
VI	$Zn(L233)^{2+}$		0.286689 (0.287384)	-2258.950626 (-545.263218)	-2259.237315 (-545.550602)
VII	$Zn(L233H)^{3+}$	2, 3	0.298733 (0.299701)	-2258.974776 (-545.292559)	-2259.273509 (-545.592260)
VIII	$Zn(L233H)^{3+}$	3, 3	0.299143 (0.300286)	-2258.970324 (-545.292779)	-2259.269467 (-545.593065)
IX	$Zn(L333)^{2+}$		0.315832 (0.316343)	-2298.266143 (-584.558706)	-2298.581975 (-584.875049)
X	$Zn(L333H)^{3+}$	3,3	0.328118 (0.329488)	-2298.295082 (-584.597420)	-2298.623200 (-584.926908)
I	$Cd(L222)^{2+}$		0.229261 (0.229730)	-5868.074573 (-449.127650)	-5868.303834 (-449.357380)
II	$Cd(L222H)^{3+}$	2,2	0.241766 (0.242192)	-5868.105039 (-449.161224)	-5868.396805 (-449.403416)
III	$Cd (L223)^{2+}$		0.257569 (0.257942)	-5907.374947 (-488.417924)	-5907.632516 (-488.675866)
IV	$Cd(L223H)^{3+}$	2, 2	0.269923 (0.270274)	-5907.411048 (-488.458579)	-5907.680971 (-488.728853)
V	$Cd(L223H)^{3+}$	2, 3	0.270381 (0.270852)	-5907.413536 (-488.461204)	-5907.683917 (-488.732056)
VI	$Cd (L233)^{2+}$		0.286061 (0.286354)	-5946.673554 (-527.706328)	-5946.959615 (-527.992682)
VII	$Cd(L233H)^{3+}$	2, 3	0.298749 (0.299161)	-5946.717779 (-527.755736)	-5947.016528 (-528.054897)
VIII	$Cd(L233H)^{3+}$	3, 3	0.299402 (0.299930)	-5946.724096 (-527.761251)	-5947.023498 (-528.061181)
IX	$Cd (L333)^{2+}$		0.314794 (0.315042)	-5985.975877 (-566.997673)	-5986.290671 (-567.312715)
X	$Cd(L333H)^{3+}$	3,3	0.328517 (0.328778)	-5986.027086 (-567.055322)	-5986.355603 (-567.384100)

[a] The data obtained at the LanL2DZ are given in parentheses.
[b] The 2,2; 2,3 or 3,3 are correspond to a secondary amine located between two ethylene arms, one ethylene and one propylene arm or two propylene arms, respectively.

Corresponding Formula used here for calculation of gas phase macrobasicities:

$$\overline{\Delta G_1} = \frac{\sum_{i=1}^{m} \Delta G_i \times S_i}{\sum_{i=1}^{m} S_i} \qquad \textbf{(eq S1)}$$

$$\overline{\Delta G_1} = \frac{\sum_{i=1}^{m} \Delta G_i \times X_i}{\sum_{i=1}^{m} X_i} \qquad \textbf{(eq S2)}$$

$$\overline{\Delta G_1} = \frac{\sum_{i=1}^{m} \Delta G_i \times S_i \times X_i}{\sum_{i=1}^{m} S_i \times X_i} \qquad \textbf{(eq S3)}$$

Where ΔG_i ,is on of the microbasicities in first protonation step of a polybasic compound and defined as the negative of the Gibbs free energy difference (sum of electronic and thermal free energies) between the initial compound and its i^{th} protonated form. The S_i is the available identical sites to undergo protonation and the x_i is population of each species and .both are defined in the text

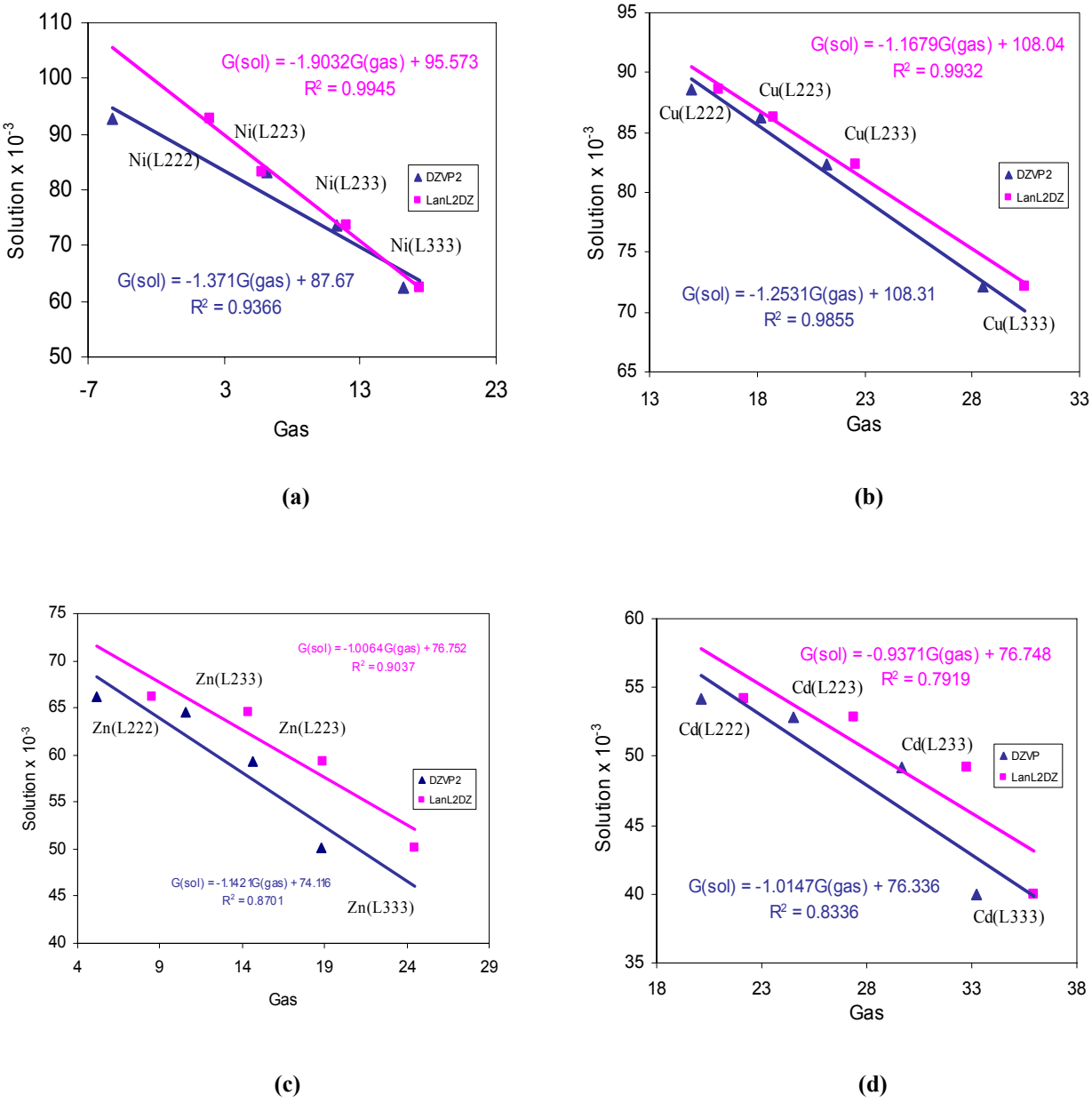


Fig. S6: Correlation of measured *G* in solution vs. calculated G in the gas phase for the first protonation step of $[NiL]^{2+}$, $[CuL]^{2+}$, $[ZnL]^{2+}$ and $[CdL]^{2+}$complexes, a, b, c and d, respectively, at the B3LYP level of theory using both the LanL2DZ and DZVP2 (DZVP for Cd^{2+}) basis sets. The data are derived from Eq (S1)

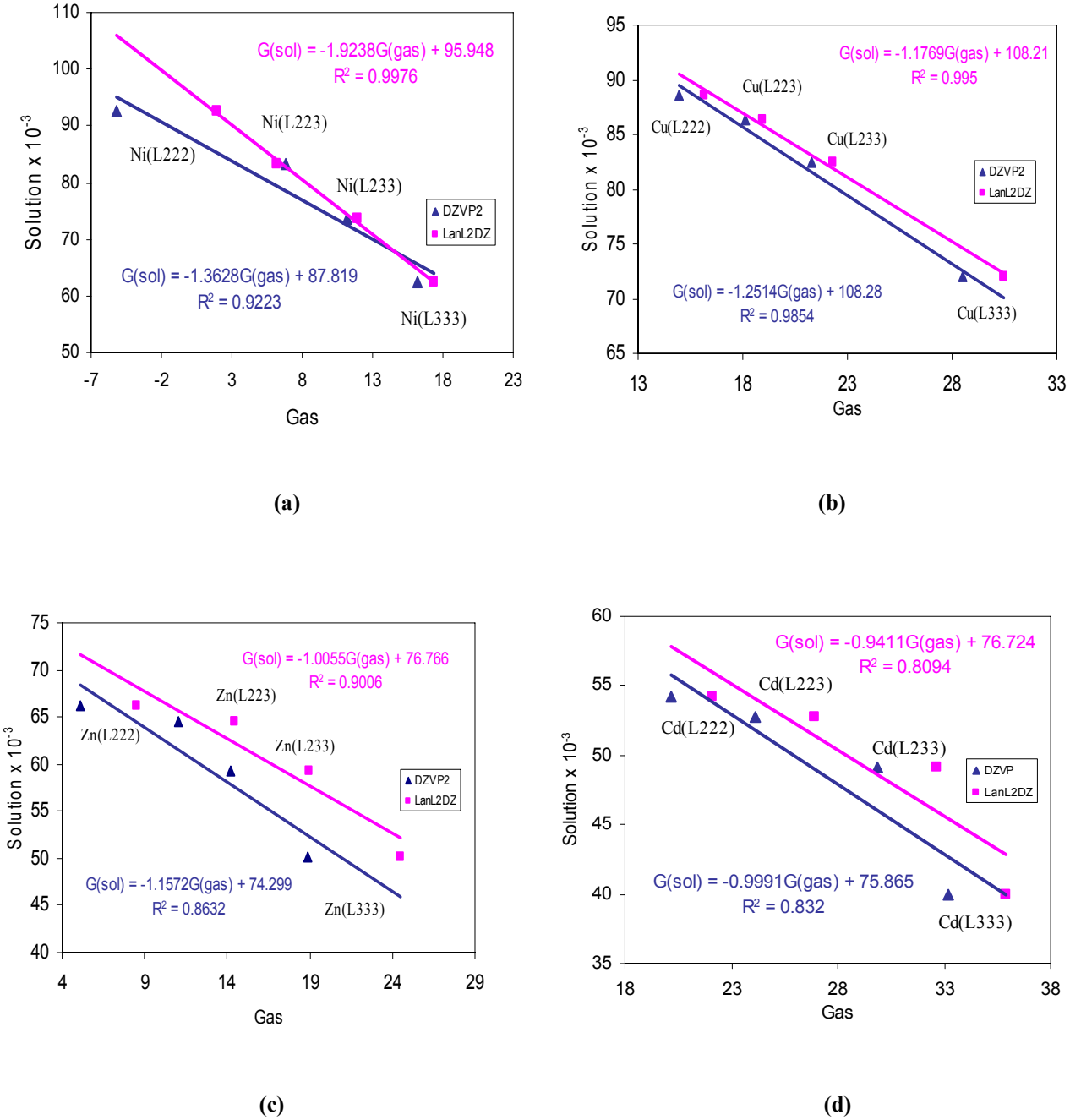
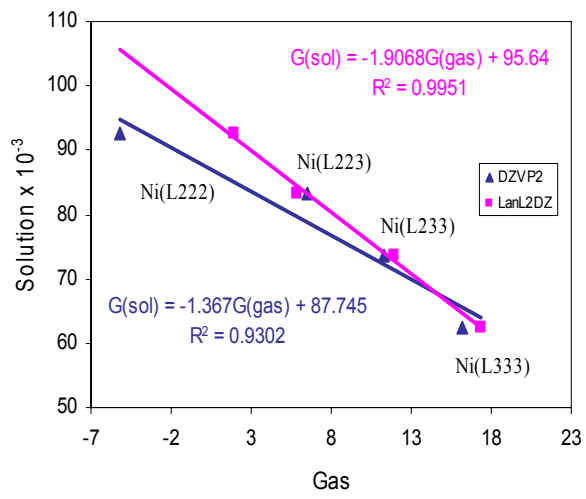
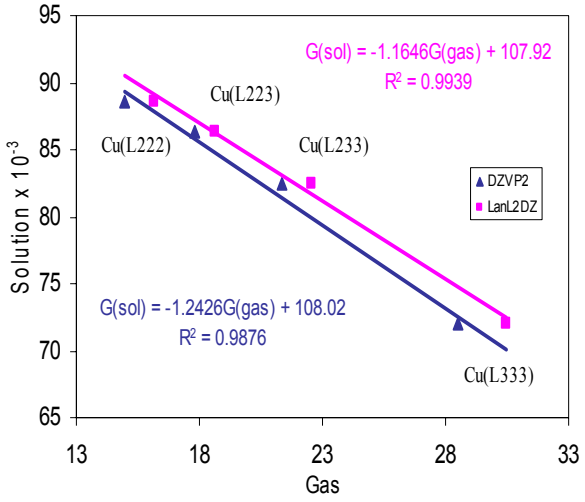


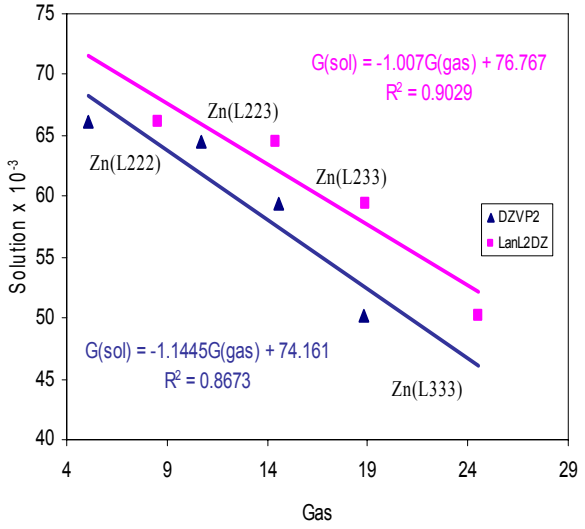
Fig. S7: Correlation of measured *G* in solution vs. calculated G in the gas phase for the first protonation step of $[NiL]^{2+}$, $[CuL]^{2+}$, $[ZnL]^{2+}$ and $[CdL]^{2+}$complexes, a, b, c and d, respectively, at the B3LYP level of theory using both the LanL2DZ and DZVP2 (DZVP for Cd^{2+}) basis sets. The data are derived from Eq (S2)



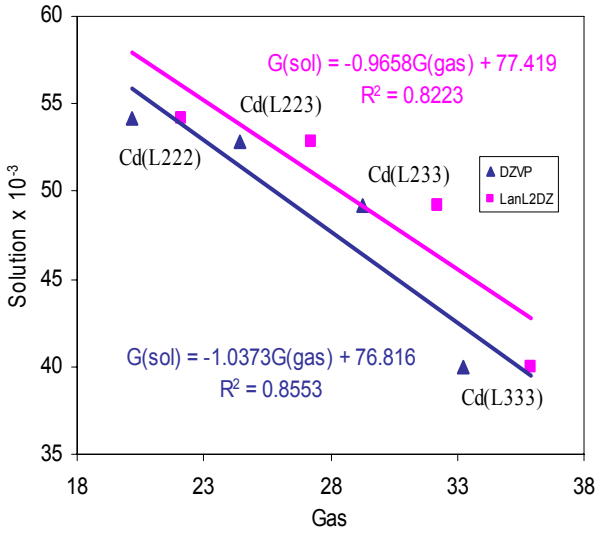
(a)



(b)



(c)



(d)

Fig. S8: Correlation of measured *G* in solution vs. calculated G in the gas phase for the first protonation step of $[NiL]^{2+}$, $[CuL]^{2+}$, $[ZnL]^{2+}$ and $[CdL]^{2+}$complexes, a, b, c and d, respectively, at the B3LYP level of theory using both the LanL2DZ and DZVP2 (DZVP for Cd^{2+}) basis sets. The data are derived from Eq (S3)

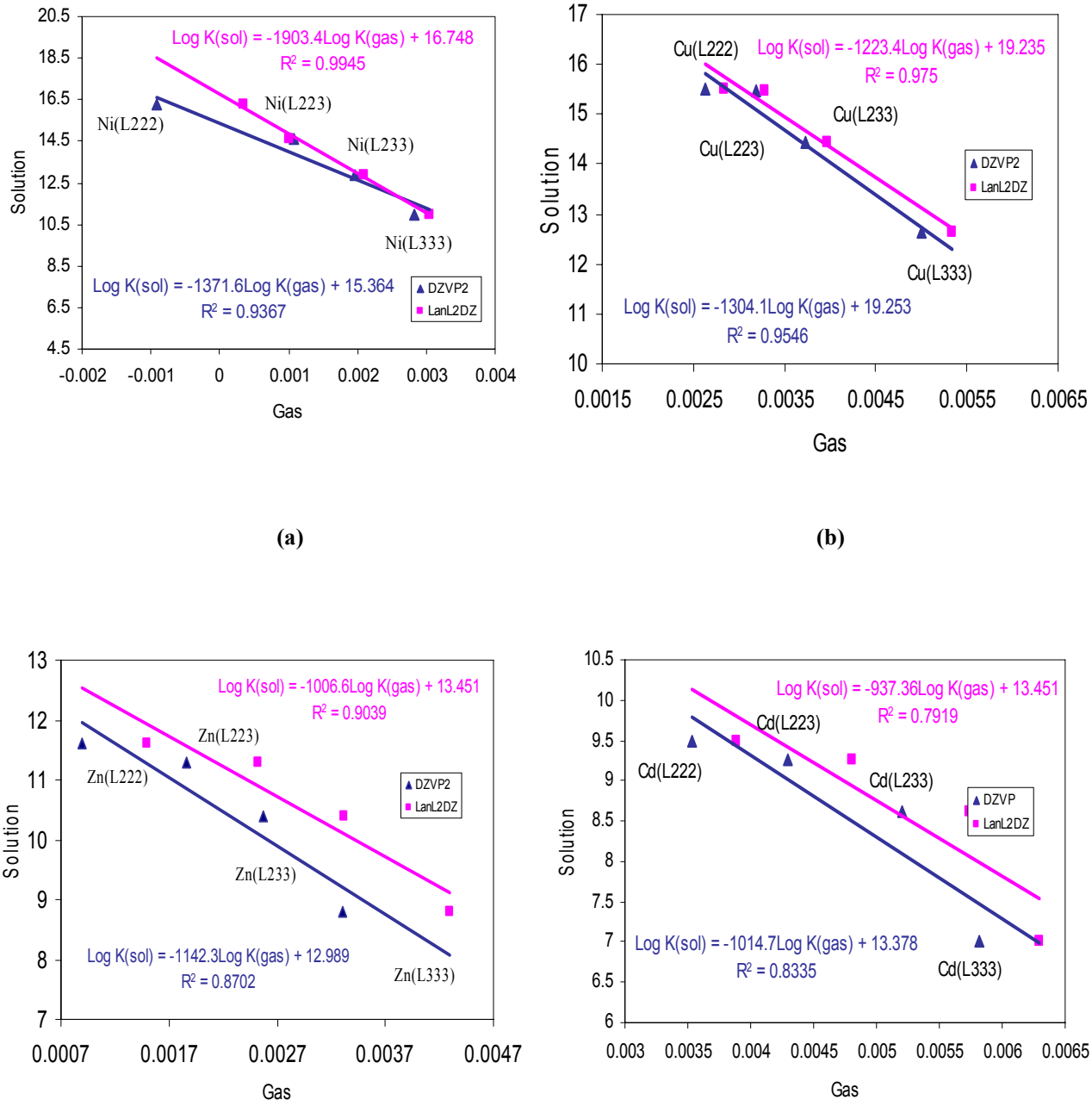


Fig. S9: Correlation of measured *Log K* in solution vs. calculated Log K in the gas phase for the first protonation step of $[NiL]^{2+}$, $[CuL]^{2+}$, $[ZnL]^{2+}$ and $[CdL]^{2+}$complexes, a, b, c and d, respectively, at the B3LYP level of theory using both the LanL2DZ and DZVP2 (DZVP for Cd^{2+}) basis sets. The K values for the gas phase were calculated from the equation $\Delta G = -RTLn\ K$, where the G values derived from Eq (S1)

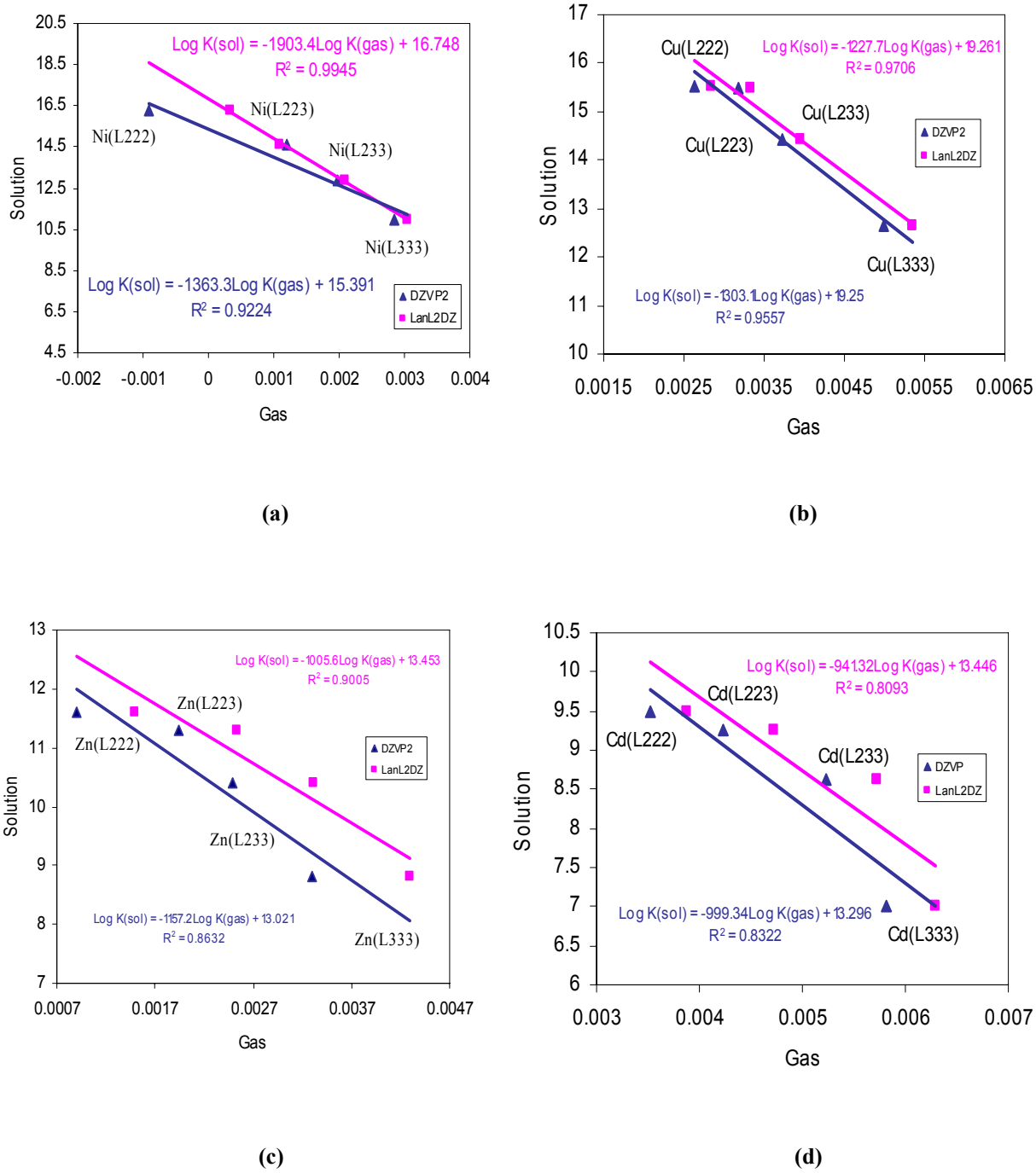
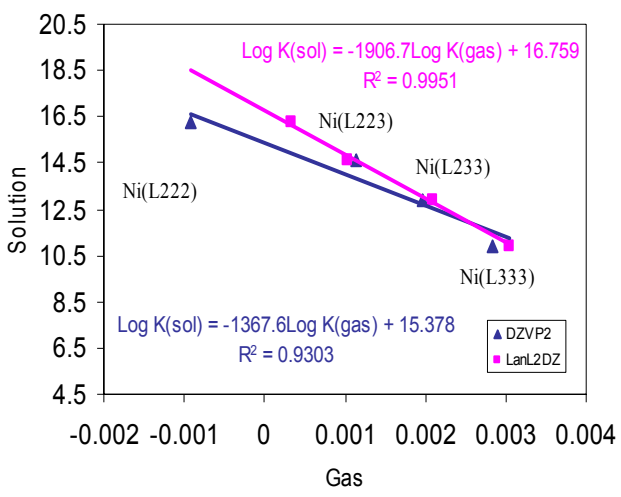
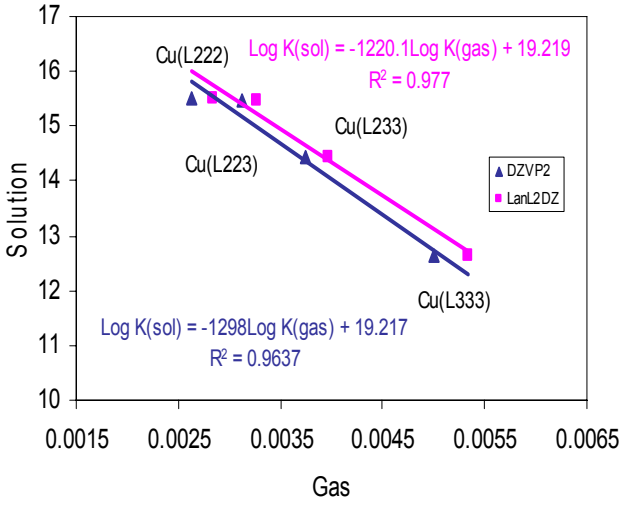


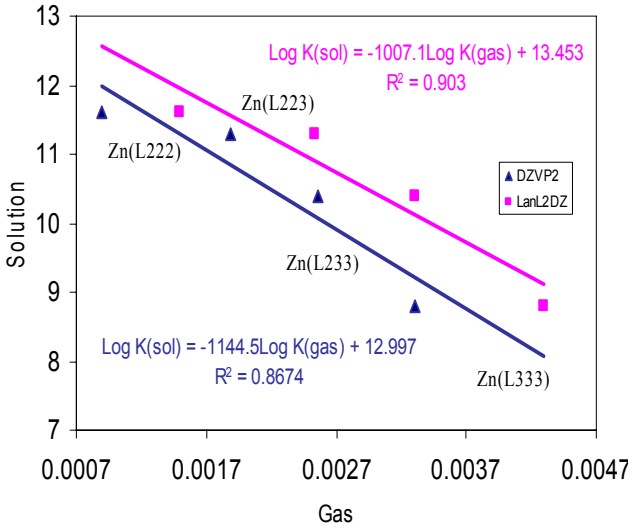
Fig. S10: Correlation of measured *Log K* in solution vs. calculated Log K in the gas phase for the first protonation step of $[NiL]^{2+}$, $[CuL]^{2+}$, $[ZnL]^{2+}$ and $[CdL]^{2+}$complexes, a, b, c and d, respectively, at the B3LYP level of theory using both the LanL2DZ and DZVP2 (DZVP for Cd^{2+}) basis sets. The K values for the gas phase were calculated from the equation $\Delta G = -RTLn\ K$, where the G values derived from Eq (S2)



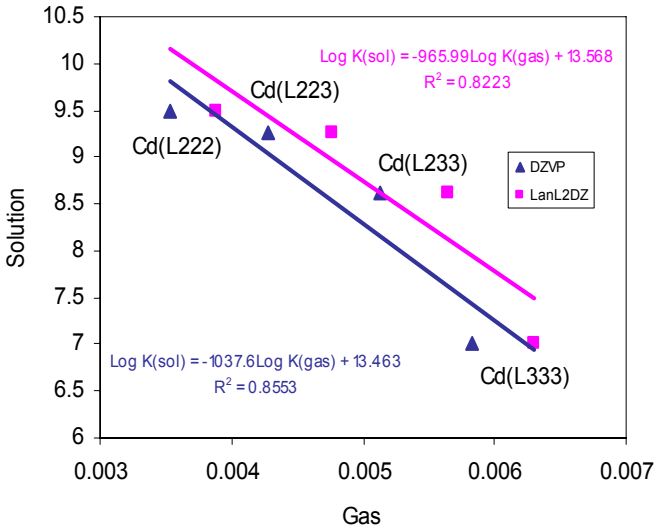
(a)



(b)



(c)



(d)

Fig. S11: Correlation of measured *Log K* in solution vs. calculated Log K in the gas phase for the first protonation step of $[NiL]^{2+}$, $[CuL]^{2+}$, $[ZnL]^{2+}$ and $[CdL]^{2+}$complexes, a, b, c and d, respectively, at the B3LYP level of theory using both the LanL2DZ and DZVP2 (DZVP for Cd^{2+}) basis sets. The K values for the gas phase were calculated from the equation $\Delta G = -RTLn\ K$, where the G values derived from Eq (S2)

Table S2:
Calculated microbasicities, $-\Delta G_i$, of the $[ML]^{2+}$ complexes at B3LYP level of theory using DZVP2 in the case of $[NiL]^{2+}$, $[CuL]^{2+}$ and $[ZnL]^{2+}$ complexes and DZVP for $[CdL]^{2+}$ complexes.[a]

No.		Protonated site[b]	$-\Delta G$	No.		Protonated site[b]	$-\Delta G$
I	$Ni(L222)^{2+}$			I	$Zn(L222)^{2+}$		
II	$Ni(L222H)^{3+}$	2,2	-5.2 (1.9)	II	$Zn(L222H)^{3+}$	2,2	5.1 (8.5)
III	$Ni(L223)^{2+}$			III	$Zn(L223)^{2+}$		
IV	$Ni(L223H)^{3+}$	2, 2	7.5 (7.0)	IV	$Zn(L223H)^{3+}$	2, 2	12.0 (14.6)
V	$Ni(L223H)^{3+}$	2, 3	5.5 (5.2)	V	$Zn(L223H)^{3+}$	2, 3	9.9 (14.3)
VI	$Ni(L233)^{2+}$			VI	$Zn(L233)^{2+}$		
VII	$Ni(L233H)^{3+}$	2, 3	11.3 (12.0)	VII	$Zn(L233H)^{3+}$	2, 3	15.5 (18.8)
VIII	$Ni(L233H)^{3+}$	3, 3	11.1 (11.9)	VIII	$Zn(L233H)^{3+}$	3, 3	13.0 (19.1)
IX	$Ni (L333)^{2+}$			IX	$Zn(L333)^{2+}$		
X	$Ni(L333H)^{3+}$	3,3	16.2 (17.4)	X	$Zn(L333H)^{3+}$	3,3	18.8 (24.5)
I	$Cu(L222)^{2+}$			I	$Cd(L222)^{2+}$		
II	$Cu(L222H)^{3+}$	2,2	15.0 (16.2)	II	$Cd(L222H)^{3+}$	2,2	20.1 (22.1)
III	$Cu (L223)^{2+}$			III	$Cd (L223)^{2+}$		
IV	$Cu(L223H)^{3+}$	2, 2	19.7 (20.1)	IV	$Cd(L223H)^{3+}$	2, 2	23.4 (26.2)
V	$Cu(L223H)^{3+}$	2, 3	17.4 (18.0)	V	$Cd(L223H)^{3+}$	2, 3	25.1 (28.0)
VI	$Cu (L233)^{2+}$			VI	$Cd (L233)^{2+}$		
VII	$Cu(L233H)^{3+}$	2, 3	21.4 (22.5)	VII	$Cd(L233H)^{3+}$	2, 3	28.3 (31.6)
VIII	$Cu(L233H)^{3+}$	3, 3	21.0 (22.8)	VIII	$Cd(L233H)^{3+}$	3, 3	32.4 (35.0)
IX	$Cu (L333)^{2+}$			IX	$Cd (L333)^{2+}$		
X	$Cu(L333H)^{3+}$	3,3	28.5 (30.5)	X	$Cd(L333H)^{3+}$	3,3	33.2 (35.9)

[a] The data in parentheses are calculated using LanL2DZ basis set.

[b] The 2,2; 2,3 or 3,3 are correspond to a secondary amine located between two ethylene arms, one ethylene and one propylene arm or two propylene arms, respectively.

Table S3:
Comparison between the experimental ΔG values for formation of $[ML]^{2+}$ complexes and calculated first macrobasicities at B3LYP level of theory using DZVP2 in the case of $[NiL]^{2+}$, $[CuL]^{2+}$ and $[ZnL]^{2+}$ complexes and DZVP for $[CdL]^{2+}$ complexes [a]

	$\Delta G(sol) \times 10^{-3}$				$\overline{\Delta G_1}$ *(gas)*			
	Ni	Cu	Zn	Cd	Ni	Cu	Zn	Cd
L222	92.66	88.56	66.19	54.20	**-5.2 (1.9)** [c,d]	**15.0 (16.2)**	**5.1 (8.5)**	**20.1 (22.1)**
L223	83.19	86.33	64.48	52.78	**6.2 (5.8)**	**18.2 (18.8)**	**10.6 (14.4)**	**24.5 (27.4)**
					6.8 (6.2)	18.1 (19.0)	11.1 (14.5)	24.1 (26.9)
					6.58 (5.9)	*17.8 (18.6)*	*10.7 (14.4)*	*24.4 (27.2)*
L233	73.49	82.39	59.34	49.18	**11.2 (11.9)**	**21.2 (22.6)**	**14.7 (18.9)**	**29.7 (32.8)**
					11.2 (11.9)	21.3 (22.6)	14.2 (18.9)	29.9 (32.6)
					11.3 (11.9)	*21.3 (22.6)*	*14.6 (18.9)*	*29.3 (32.2)*
L333	62.36	72.06	50.21	40.00	**16.2 (17.4)**	**28.5 (30.5)**	**18.8 (24.5)**	**33.2 (35.9)**

[a] The data in parentheses are calculated using LanL2DZ basis set

[b] The experimental Kf values reported in Ref [5c] were puted in equation G=-RTLnK to calculate the experimental ΔG values

[c] The data were derived from Eq (S1) are given as bold, those were derived with Eq(S2) are in plain text and those were derived from Eq(S3) are in italic.

[d] Note that for the symmetrical complexes ($[ML222]^{2+}$ and $[ML333]^{2+}$) there is only one microbasicity and the data derived from the eqs. (1), (2) and (3) are all equal ($G_i = \overline{\Delta G_1}$)

Table S4:
Comparison between calculated protonation macroconstants of $[ML]^{2+}$ complexes calculated at B3LYP level of theory using DZVP2 in the case of $[NiL]^{2+}$, $[CuL]^{2+}$ and $[ZnL]^{2+}$ complexes and DZVP for $[CdL]^{2+}$ complexes [a] and their measured G in solution.

	Log K_f(sol)				*Log K(gas) × 10³*			
	Ni	Cu	Zn	Cd	Ni	Cu	Zn	Cd
L222	16.24	15.52	11.6	9.5	**-0.9 (0.3)** [c,d]	**2.6 (2.8)**	**0.9 (1.5)**	**3.5 (3.9)**
L223	14.58	15.48	11.3	9.25	**1.1 (1.0)**	**3.2 (3.3)**	**1.8 (2.5)**	**4.3 (4.8)**
					1.2 (1.1)	3.2 (3.3)	1.9 (2.5)	4.2 (4.7)
					1.1 (1.0)	*3.1 (3.3)*	*1.9 (2.5)*	*4.3 (4.8)*
L233	12.88	14.44	10.4	8.62	**2.0 (2.1)**	**3.7 (4.0)**	**2.6 (3.3)**	**5.2 (5.7)**
					2.0 (2.1)	3.7 (4.0)	2.5 (3.3)	5.2 (5.7)
					2.0 (2.1)	*3.7 (4.0)*	*2.6 (3.3)*	*5.1 (5.6)*
L333	10.93	12.63	8.8	7.01	**2.8 (3.0)**	**5.0 (5.3)**	**3.3 (4.3)**	**5.8 (6.3)**

[a] The data in parentheses are calculated using LanL2DZ basis set

[b] The experimental value were derived from Ref [5c].

[c] The data were derived from Eq (S1) are given as bold, those were derived with Eq(S2) are in plain text and those were derived from Eq(S3) are in italic.

[d] Note that for the symmetrical complexes ($[ML222]^{2+}$ and $[ML333]^{2+}$) there is only one microbasicity and the data derived from the eqs. (1), (2) and (3) are all equal ($G_i = \overline{\Delta G_1}$)

Table S5:
Calculated Gibbs free energies, *G, Thermal correction to Gibbs Free Energy, Gcorr, and* Maxwell-Boltzmann distribution , X_i, for $[NiL]^{2+}$, $[CuL]^{2+}$, $[ZnL]^{2+}$ and $[CdL]^{2+}$ complexes and their possible protonated forms at B3LYP level of theory using DZVP2 basis set for NI^{2+}, Cu^{2+} and Zn^{2+} and DZVP for Cd^{2+} .[a]

No.		Protonated site[b]	*G (Hartree)*	G_{corr} *(Hartree)*	G_{corr}*(KJ/mol)*	X_i
I	$Ni(L222)^{2+}$		-1909.338749 (-570.418182)	0.194674 (0.195463)	510.6 (512.6)	
II	$Ni(L222H)^{3+}$	2,2	-1909.330420 (-570.421252)	0.205335 (0.205824)	538.5 (539.8)	1 (1)[b]
III	$Ni(L223)^{2+}$		-1948.653575 (-609.715523)	0.222273 (0.223003)	583.0 (584.9)	
IV	$Ni(L223H)^{3+}$	2, 2	-1948.665555 (-609.726743)	0.231485 (0.232347)	607.1 (609.4)	0.64402 (0.60955)
V	$Ni(L223H)^{3+}$	2, 3	-1948.662415 (-609.723788)	0.232045 (0.232768)	608.6 (610.5)	0.35597 (0.39044)
VI	$Ni(L233)^{2+}$		-1987.963818 (-649.008086)	0.248050 (0.249049)	650.6 (653.2)	
VII	$Ni(L233H)^{3+}$	2, 3	-1987.981835 (-649.027136)	0.258883 (0.259282)	679.0 (680.0)	0.64572 (0.76489)
VIII	$Ni(L233H)^{3+}$	3, 3	-1987.981521 (-649.027100)	0.259450 (0.260397)	680.5 (683.0)	0.35427 (0.23510)
IX	$Ni (L333)^{2+}$		-2027.272657 (-688.299232)	0.275868 (0.276568)	723.5 (725.4)	
X	$Ni(L333H)^{3+}$	3,3	-2027.298459 (-688.326955)	0.285570 (0.287212)	749.0 (753.3)	1 (1)
I	$Cu(L222)^{2+}$		-2041.452448 (-597.224129)	0.192682 (0.193781)	505.4 (508.2)	
II	$Cu(L222H)^{3+}$	2,2	-2041.476326 (-597.249927)	0.204135 (0.204444)	535.4 (536.2)	1 (1)
III	$Cu (L223)^{2+}$		-2080.768859 (-636.524035)	0.220667 (0.221579)	578.8 (581.1)	
IV	$Cu(L223H)^{3+}$	2, 2	-2080.800235 (-636.556130)	0.231368 (0.231943)	606.8 (608.3)	0.31617 (0.43035)
V	$Cu(L223H)^{3+}$	2, 3	-2080.796559 (-636.552808)	0.230639 (0.231678)	604.9 (607.6)	0.68382 (0.56964)
VI	$Cu (L233)^{2+}$		-2120.083734 (-675.821112)	0.247120 (0.247962)	648.1 (650.4)	
VII	$Cu(L233H)^{3+}$	2, 3	-2120.117826 (-675.857013)	0.257939 (0.258849)	676.5 (678.9)	0.78125 (0.72581)
VIII	$Cu(L233H)^{3+}$	3, 3	-2120.117172 (-675.857413)	0.259142 (0.259769)	679.7 (681.3)	0.21874 (0.27418)
IX	$Cu (L333)^{2+}$		-2159.397134 (-715.117255)	0.274269 (0.275182)	719.4 (721.7)	
X	$Cu(L333H)^{3+}$	3,3	-2159.442569 (-715.165825)	0.286845 (0.287812)	752.3 (754.9)	1 (1)
I	$Zn(L222)^{2+}$		-2180.360171 (-466.712390)	0.195953 (0.196713)	513.9 (515.9)	
II	$Zn(L222H)^{3+}$	2,2	-2180.368312 (-466.725991)	0.206413 (0.207321)	541.4 (543.8)	1 (1)
III	$Zn(L223)^{2+}$		-2219.673908 (-506.006550)	0.222644 (0.223517)	583.9 (586.2)	
IV	$Zn(L223H)^{3+}$	2, 2	-2219.692971 (-506.029756)	0.233248 (0.234112)	611.8 (614.0)	0.56731 (0.67087)
V	$Zn(L223H)^{3+}$	2, 3	-2219.689722 (-506.029347)	0.233504 (0.234785)	612.4 (615.8)	0.43268 (0.32912)
VI	$Zn(L233)^{2+}$		-2258.988461 (-545.301113)	0.248853 (0.249488)	652.7 (654.4)	
VII	$Zn(L233H)^{3+}$	2, 3	-2259.013154 (-545.331074)	0.260355 (0.261186)	682.9 (685.0)	0.46856 (0.57482)
VIII	$Zn(L233H)^{3+}$	3, 3	-2259.009232 (-545.331594)	0.260236 (0.261471)	682.5 (685.8)	0.53143 (0.42517)
IX	$Zn(L333)^{2+}$		-2298.304961 (-584.597906)	0.277014 (0.277143)	726.6 (726.9)	
X	$Zn(L333H)^{3+}$	3,3	-2298.334997 (-584.636976)	0.288202 (0.289932)	755.9 (760.4)	1 (1)
I	$Cd(L222)^{2+}$		-5868.109393 (-449.162457)	0.194441 (0.194924)	510.0 (511.2)	
II	$Cd(L222H)^{3+}$	2,2	-5868.141494 (-449.197749)	0.205311 (0.205667)	538.5 (539.4)	1 (1)
III	$Cd (L223)^{2+}$		-5907.411373 (-488.454420)	0.221142 (0.221446)	580.0 (580.8)	
IV	$Cd(L223H)^{3+}$	2, 2	-5907.448610 (-488.496254)	0.232362 (0.232600)	609.4 (610.1)	0.55166 (0.61333)
V	$Cd(L223H)^{3+}$	2, 3	-5907.451360 (-488.499020)	0.232558 (0.233036)	609.9 (611.2)	0.44833 (0.38666)
VI	$Cd (L233)^{2+}$		-5946.712019 (-527.744968)	0.247596 (0.247714)	649.4 (649.7)	
VII	$Cd(L233H)^{3+}$	2, 3	-5946.757177 (-527.795354)	0.259351 (0.259543)	680.2 (680.7)	0.62357 (0.70183)
VIII	$Cd(L233H)^{3+}$	3, 3	-5946.763671 (-527.800829)	0.259828 (0.260352)	681.5 (682.9)	0.37642 (0.29816)
IX	$Cd (L333)^{2+}$		-5986.014665 (-567.039147)	0.276006 (0.273569)	723.9 (717.5)	
X	$Cd(L333H)^{3+}$	3,3	-5986.067612 (-567.096404)	0.287991 (0.287696)	755.3 (754.6)	1 (1)

[a] The data in parentheses are calculated using LanL2DZ basis set
[b] Note that for the symmetrical complexes ($[ML222]^{2+}$ and $[ML333]^{2+}$) there is only one microspecies.

Cartesian coordinate representation of the optimized molecular structure of the $[ZnL]^{2+}$, $[CuL]^{2+}$, $[CdL]^{2+}$ and $[NiL]^{2+}$ complexes of Triazacycloalkanes ([X] ane N_3, X = 9 – 12) and their possible protonated forms at B3LYP/LanL2DZ and B3LYP/DGDZVP2 level of theory

B3LYP/LanL2DZ

$Cu(L222)^{2+}$(I)

N	0.516441	-0.705162	1.784516
C	0.516441	0.816497	1.784516
C	-0.846277	-1.373302	1.784516
Cu	1.102495	-1.290664	-0.092844
C	1.428680	1.360844	0.669114
N	1.165065	0.628153	-0.642821
N	-0.812107	-1.435237	-0.806630
C	-1.635914	-1.183756	0.448660
C	-0.167097	0.943534	-1.326046
C	-0.865347	-0.328934	-1.848129
H	1.071896	-1.065731	2.568003
H	0.868373	1.192003	2.750992
H	-0.514360	1.163742	1.666975
H	-1.468121	-0.974997	2.597624
H	-0.681791	-2.437806	1.993091
H	2.485353	1.210407	0.917432
H	1.269060	2.437806	0.523778
H	1.947298	0.783509	-1.294488
H	-1.087449	-2.322887	-1.239665
H	-2.051164	-0.173891	0.391691
H	-2.485353	-1.874789	0.472264
H	0.015556	1.631376	-2.159408
H	-0.791978	1.469822	-0.600609
H	-1.903610	-0.088686	-2.109044
H	-0.374741	-0.708477	-2.750992

$Cu(L222H)^{3+}$(II)

N	0.809004	-0.654621	1.655316
C	0.809004	0.890711	1.655316
C	-0.563663	-1.353848	1.655316
Cu	2.080271	-1.198304	0.178620
C	1.562145	1.455533	0.428650
N	1.496101	0.482994	-0.757096
C	-1.673840	-0.807552	0.738801
N	-1.694481	-1.255061	-0.740890
C	0.174571	0.411981	-1.540885
C	-0.476438	-0.989599	-1.660778
H	1.287720	-0.986496	2.511483
H	1.297635	1.235895	2.572883
H	-0.225102	1.236853	1.701969
H	-0.950524	-1.236679	2.681247
H	-0.397857	-2.431949	1.526575
H	2.624716	1.609752	0.654577

H	1.160329	2.431949	0.125530
H	2.245808	0.735943	-1.422754
H	-1.736375	0.282371	0.741392
H	-2.624716	-1.167768	1.152658
H	-1.903048	-2.268580	-0.788071
H	-2.520160	-0.793327	-1.164997
H	0.404047	0.754637	-2.556652
H	-0.511309	1.151415	-1.113447
H	-0.853083	-1.126893	-2.681247
H	0.238303	-1.805948	-1.495096

$Cu(L223)^{2+}$(III)

N	0.409165	-0.283911	-1.934555
C	0.409165	1.259490	-1.934555
C	-0.974738	-0.932334	-1.934555
Cu	1.116625	-0.634315	-0.110285
C	0.922773	1.922668	-0.614633
N	0.657910	0.437676	1.487085
C	-0.978685	-2.210630	-1.077029
N	-0.373707	-1.920698	0.288775
C	0.156184	1.687164	0.730412
C	-1.254206	-1.176276	1.283891
C	-0.389945	-0.348463	2.256197
H	0.947806	-0.623520	-2.738249
H	-0.603948	1.604932	-2.166273
H	1.062188	1.592259	-2.747367
H	-1.286623	-1.167204	-2.957928
H	-1.685167	-0.198961	-1.541956
H	0.888862	3.002639	-0.811850
H	2.002677	1.723282	-0.473479
H	1.415462	0.710304	2.123400
H	-0.379759	-3.002639	-1.539076
H	-2.002677	-2.589404	-0.961380
H	-0.011587	-2.786588	0.709563
H	-0.919073	1.573350	0.559327
H	0.291072	2.556017	1.382877
H	-1.866167	-1.894505	1.842606
H	-1.936941	-0.538986	0.715065
H	-1.027463	0.323006	2.844089
H	0.142536	-0.999838	2.957928

$Cu(L223H)^{3+}$(IV)

N	0.638121	-0.467966	-1.786250
C	0.638121	1.066898	-1.786250
C	-0.728559	-1.169573	-1.786250
Cu	1.931851	-1.077502	-0.367727
C	1.768011	1.683452	-0.928254
N	1.443896	0.154753	1.144307
C	-1.113865	-1.964046	-0.517336
N	-1.837681	-1.190025	0.605106
C	1.539158	1.590750	0.604984
C	0.185804	-0.184015	1.952423

C	-1.174603	0.043799	1.258345
H	1.139502	-0.774849	-2.638706
H	-0.344609	1.416601	-1.459000
H	0.772896	1.393358	-2.827791
H	-0.706253	-1.902423	-2.601755
H	-1.492847	-0.430401	-2.057298
H	1.827942	2.752598	-1.174712
H	2.756572	1.283827	-1.213977
H	2.243994	-0.005352	1.784020
H	-0.258332	-2.476082	-0.059662
H	-1.815790	-2.752598	-0.817044
H	-2.756572	-0.876231	0.243371
H	-2.061995	-1.876154	1.348545
H	0.631683	2.131013	0.889435
H	2.387857	2.072254	1.108532
H	0.210343	0.482910	2.827791
H	0.293988	-1.201616	2.349466
H	-1.891623	0.372741	2.019938
H	-1.141679	0.829330	0.501223

$Cu(L223H)^{3+}$(V)

N	1.836824	-0.659424	-1.381433
C	1.836824	0.897818	-1.381433
C	0.479722	-1.417882	-1.381433
C	1.355028	1.580566	-0.080314
C	0.041333	-2.133503	-0.082112
N	-0.732518	-1.365889	1.002400
C	-0.185176	1.856892	0.027982
Cu	0.263795	-0.055583	2.183156
N	-0.817350	1.408471	1.340228
C	-2.012632	-0.639227	0.527370
C	-2.175823	0.713313	1.242069
H	2.315939	-0.924541	-2.261012
H	2.453566	-1.004413	-0.628828
H	1.252590	1.210080	-2.253573
H	2.881092	1.173435	-1.568674
H	0.596026	-2.216967	-2.122794
H	-0.267681	-0.733262	-1.786779
H	1.887128	2.537783	-0.024265
H	1.741158	1.020925	0.798121
H	0.881749	-2.644069	0.407794
H	-0.639231	-2.935897	-0.410927
H	-1.011673	-2.088965	1.689119
H	-0.735832	1.375666	-0.782747
H	-0.367028	2.935897	-0.058855
H	-0.867005	2.199276	2.004717
H	-2.880925	-1.275865	0.734551
H	-1.955229	-0.519505	-0.555255
H	-2.881092	1.359780	0.699794
H	-2.565753	0.598919	2.261012

$Cu(L233)^{2+}$(VI)

N	0.405320	-0.092379	-2.381424
C	0.405320	1.425766	-2.381424
C	-0.977589	-0.780838	-2.381424
Cu	0.971066	-0.674253	-0.592947
C	-1.021159	-2.126873	-1.581463
N	0.931771	1.221186	0.073496
C	0.095415	1.954297	-0.967915
N	0.109836	-1.788521	0.763692
C	-1.192269	-2.074951	-0.025995
C	-0.085436	-1.153389	2.138453
C	0.434955	1.320704	1.506613
C	0.799026	0.092105	2.372942
H	0.949311	-0.431550	-3.182560
H	-0.328472	1.818541	-3.095472
H	1.397865	1.749957	-2.713876
H	-1.258162	-0.975719	-3.422205
H	-1.706031	-0.072402	-1.972845
H	-0.178718	-2.779853	-1.868405
H	-1.906642	-2.659699	-1.952550
H	1.911231	1.538017	0.030323
H	-0.955504	1.798027	-0.705181
H	0.290531	3.032544	-0.914910
H	0.617388	-2.673831	0.886350
H	-1.596366	-3.032544	0.321047
H	-1.911231	-1.295601	0.246643
H	0.141848	-1.903778	2.903407
H	-1.143076	-0.890023	2.246123
H	-0.650753	1.459858	1.475614
H	0.873341	2.224007	1.951554
H	1.865212	-0.159678	2.271017
H	0.666654	0.386493	3.422205

$Cu(L233H)^{3+}$(VII)

N	0.401370	-0.144467	-1.831485
C	0.401370	1.393837	-1.831485
C	-0.976498	-0.819390	-1.831485
Cu	1.606488	-1.194652	-0.594674
C	-0.911057	-2.303047	-1.411220
C	-0.277862	2.171980	-0.676516
N	0.307486	-1.788150	0.811638
N	0.629819	2.645966	0.494440
C	-0.813863	-2.564683	0.123595
C	-0.146972	-0.571023	1.597468
C	0.530986	1.934095	1.874397
C	0.989156	0.457289	1.876879
H	0.855514	-0.403358	-2.727058
H	-0.145174	1.677812	-2.744017
H	1.436067	1.724815	-1.990651
H	-1.365234	-0.759395	-2.859744
H	-1.655993	-0.246547	-1.195514
H	-0.103848	-2.830766	-1.947689
H	-1.832881	-2.794570	-1.749480
H	-1.135865	1.660387	-0.237308

H	-0.666885	3.092887	-1.124458
H	0.861063	-2.419820	1.416758
H	0.378589	3.633276	0.680244
H	1.618502	2.670305	0.197991
H	-0.635255	-3.633276	0.284879
H	-1.756725	-2.292536	0.611937
H	-0.566613	-0.932332	2.547763
H	-0.975571	-0.129601	1.039739
H	-0.502776	2.051871	2.215882
H	1.169235	2.525468	2.540048
H	1.832881	0.339390	1.166979
H	1.432113	0.258733	2.859744

$Cu(L233H)^{3+}$(VIII)

N	1.249396	-0.521384	-2.307185
C	1.249396	1.010365	-2.307185
C	-0.093146	-1.273107	-2.307185
Cu	2.404356	-0.927871	-0.702921
C	-0.695644	-1.621344	-0.912393
N	1.997752	0.887362	0.094782
C	1.036228	1.552510	-0.890995
C	-1.828884	-0.682128	-0.409276
C	1.582980	0.918195	1.571527
N	-1.942703	-0.624654	1.131545
C	0.463110	-0.041969	2.061967
C	-1.030360	0.386108	1.880446
H	1.768396	-0.837469	-3.143612
H	0.467494	1.376837	-2.985262
H	2.211780	1.335552	-2.721240
H	0.091465	-2.203610	-2.853115
H	-0.792450	-0.679529	-2.914089
H	0.116065	-1.690102	-0.172853
H	-1.100839	-2.637632	-0.986150
H	2.915683	1.363448	0.035389
H	0.023869	1.365976	-0.539291
H	1.203346	2.637632	-0.872420
H	-2.794869	-1.042628	-0.778871
H	-1.726386	0.353462	-0.743194
H	1.316441	1.964678	1.795481
H	2.493107	0.703502	2.144009
H	-2.915683	-0.348371	1.351222
H	-1.826693	-1.568737	1.535526
H	0.643075	-1.066577	1.707045
H	0.636229	-0.107935	3.143612
H	-1.492121	0.499776	2.866624
H	-1.151991	1.342847	1.364229

$Cu(L333)^{2+}$(IX)

N	-0.309695	-0.000148	-2.104533
C	-0.309695	1.526518	-2.104533

C	-1.718156	-0.589114	-2.104533
Cu	0.794842	-0.734411	-0.604102
C	1.008690	2.197012	-1.662335
C	-1.829284	-2.062118	-1.655955
N	1.862894	0.697907	0.185515
N	-0.116901	-2.267157	0.192564
C	1.320097	2.072583	-0.154524
C	-1.594705	-2.295260	-0.147104
C	0.224504	-1.975415	1.672373
C	1.729337	0.273023	1.666431
C	0.395461	-0.461076	2.030062
H	0.192376	-0.334322	-2.940412
H	-1.126795	1.846175	-1.449374
H	-0.556662	1.852876	-3.124413
H	-2.112616	-0.491803	-3.125590
H	-2.329548	0.044295	-1.453382
H	0.903610	3.264792	-1.893145
H	1.859389	1.849817	-2.266969
H	-1.181287	-2.716112	-2.257781
H	-2.855212	-2.377134	-1.885564
H	2.855212	0.671552	-0.078106
H	0.288431	-3.174256	-0.067766
H	0.417135	2.240324	0.443937
H	2.057235	2.828310	0.142824
H	-2.009368	-3.264792	0.154515
H	-2.096197	-1.523363	0.448134
H	1.141539	-2.527643	1.908677
H	-0.579510	-2.391559	2.290424
H	1.810601	1.175674	2.283066
H	2.590132	-0.364381	1.899927
H	0.336162	-0.418690	3.125590
H	-0.474127	0.120061	1.685310

Cu(L333H)$^{3+}$(X)

N	2.340449	-1.745825	-1.373039
C	2.340449	-0.198941	-1.373039
C	0.973036	-2.491873	-1.373039
C	2.162679	0.410570	0.051595
C	0.075773	-2.302882	-0.119932
C	1.255490	1.677069	0.060573
C	-0.919828	-1.113654	-0.229446
N	0.465151	1.853931	1.355022
N	-1.424612	-0.599484	1.109987
Cu	0.018516	0.130489	2.293462
C	-2.463763	0.521751	1.027261
C	-0.859907	2.601509	1.209542
C	-1.950225	1.844078	0.413711
H	2.819774	-2.047578	-2.239602
H	2.924634	-2.097764	-0.597611
H	1.551383	0.103156	-2.068437
H	3.296357	0.109829	-1.807598

H	1.237483	-3.549695	-1.474396
H	0.461521	-2.190099	-2.293462
H	3.145640	0.644471	0.475161
H	1.718845	-0.351428	0.711238
H	0.697238	-2.244299	0.787525
H	-0.492932	-3.234721	-0.011781
H	0.529790	1.650955	-0.754905
H	1.859195	2.584848	-0.075767
H	-1.803585	-1.428023	-0.804392
H	-0.487181	-0.263452	-0.758157
H	1.050796	2.349576	2.050369
H	-1.831939	-1.384295	1.648850
H	-2.861615	0.670692	2.039172
H	-3.296357	0.154536	0.405878
H	-0.650479	3.549695	0.687837
H	-1.201287	2.859899	2.219768
H	-2.816590	2.518620	0.380473
H	-1.664446	1.711286	-0.635706

B3LYP/DZVP2
$Cu(L222)^{2+}$(I)

N	1.287512	0.861527	0.377603
C	1.774374	-0.172753	-0.606598
C	0.397340	1.937420	-0.173710
Cu	-0.098740	-0.054431	1.564777
C	1.502134	-1.586324	-0.074477
N	0.095378	-1.686374	0.461558
N	-1.674874	0.524153	0.404639
C	-1.011204	1.429918	-0.602902
C	-1.011333	-1.676612	-0.573214
C	-2.183097	-0.780774	-0.145159
H	2.079230	1.302365	0.846898
H	2.846386	-0.053662	-0.777646
H	1.280661	-0.001394	-1.564777
H	0.860586	2.415509	-1.044144
H	0.307931	2.700076	0.606172
H	2.174373	-1.823538	0.754484
H	1.652732	-2.340478	-0.855110
H	0.015383	-2.521417	1.049569
H	-2.448173	1.015284	0.853828
H	-0.952460	0.902864	-1.555912
H	-1.635883	2.310806	-0.767746
H	-1.363418	-2.700076	-0.726309
H	-0.577218	-1.338387	-1.514111
H	-2.846386	-0.618340	-1.000617
H	-2.767909	-1.255370	0.646748

$Cu(L222H)^{3+}$(II)

N	-0.793001	1.640723	-0.643760
C	-0.780132	1.633716	0.887341

C	0.558983	1.652772	-1.346090
Cu	-2.043792	0.181367	-1.187562
C	-1.549801	0.418288	1.437593
N	-1.477620	-0.751639	0.472823
C	1.672081	0.737952	-0.821312
N	1.683215	-0.732558	-1.244147
C	-0.176063	-1.544357	0.414752
C	0.496508	-1.664667	-0.969873
H	-1.263014	2.501204	-0.957475
H	-1.246599	2.555214	1.243852
H	0.255058	1.651566	1.224949
H	0.946277	2.674280	-1.222939
H	0.384647	1.532667	-2.421156
H	-2.612195	0.651842	1.560984
H	-1.175010	0.112776	2.421156
H	-2.223711	-1.409751	0.732205
H	1.762425	0.752956	0.264115
H	2.612195	1.143320	-1.209622
H	1.892755	-0.795271	-2.251433
H	2.515555	-1.142927	-0.794409
H	-0.426461	-2.559332	0.734623
H	0.503879	-1.141049	1.169941
H	0.902601	-2.674280	-1.079193
H	-0.209446	-1.542238	-1.798057

$Cu(L223)^{2+}$(III)

N	0.809131	1.325447	-0.518023
C	2.019784	0.663739	0.141711
C	-0.241593	1.846538	0.440295
Cu	-0.033101	-0.239601	-1.384425
C	2.149269	-0.868663	-0.093709
N	-0.097682	-2.028827	-0.577471
C	-1.648151	1.632627	-0.129955
N	-1.803803	0.206242	-0.587783
C	1.043541	-1.837830	0.421531
C	-2.012131	-0.837680	0.480094
C	-1.474107	-2.195311	0.006921
H	1.131947	2.092894	-1.107451
H	1.990450	0.884766	1.210975
H	2.916768	1.135230	-0.263783
H	-0.080104	2.907118	0.647635
H	-0.121681	1.312914	1.384425
H	3.077112	-1.151816	0.415792
H	2.368631	-1.079489	-1.154178
H	0.113233	-2.835665	-1.166530
H	-1.820319	2.268137	-1.001999
H	-2.409851	1.874517	0.619076
H	-2.550796	0.145383	-1.284648
H	0.615196	-1.481405	1.360132
H	1.485516	-2.817107	0.618272
H	-3.077112	-0.913399	0.718394
H	-1.497659	-0.499185	1.380502
H	-1.465080	-2.907118	0.837931

H	-2.107898	-2.609154	-0.781277

Cu(L223H)$^{3+}$(IV)

N	-0.633267	-1.753831	-0.482897
C	-0.637568	-1.777151	1.038825
C	0.722809	-1.772865	-1.173192
Cu	-1.902303	-0.342304	-1.086006
C	-1.754935	-0.918969	1.659258
N	-1.425209	1.138164	0.143834
C	1.127032	-0.516856	-1.965291
N	1.821248	0.609619	-1.199867
C	-1.518713	0.605635	1.569268
C	-0.190508	1.953374	-0.192319
C	1.176748	1.279344	0.015650
H	-1.127080	-2.602780	-0.789432
H	0.346104	-1.465670	1.392998
H	-0.782474	-2.819716	1.346904
H	0.692064	-2.583182	-1.907065
H	1.481066	-2.051319	-0.434792
H	-1.816805	-1.168865	2.724722
H	-2.741934	-1.195784	1.256694
H	-2.218450	1.780188	0.000873
H	0.290813	-0.070463	-2.513572
H	1.852719	-0.824949	-2.724722
H	2.741934	0.266505	-0.887224
H	2.051688	1.338250	-1.892086
H	-0.608972	0.884018	2.103578
H	-2.360129	1.115678	2.049960
H	-0.215376	2.819716	0.481313
H	-0.310783	2.357167	-1.202795
H	1.889603	2.056451	0.305953
H	1.173742	0.546023	0.821587

Cu(L223H)$^{3+}$(V)

N	2.329593	0.166449	-0.793461
C	2.111970	-1.301286	-0.384616
C	1.617543	1.304398	-0.041797
C	0.731600	-1.918657	-0.679241
C	0.428023	2.003288	-0.723325
N	-0.965920	1.405087	-0.638559
C	-0.363471	-1.763054	0.426580
Cu	-1.420006	-0.201017	-1.748550
N	-1.678855	-1.207897	-0.067615
C	-1.483130	1.120981	0.773921
C	-2.338801	-0.149795	0.787309
H	3.337810	0.326749	-0.652979
H	2.208534	0.266771	-1.809148
H	2.373314	-1.369114	0.674290
H	2.872968	-1.850373	-0.945633
H	2.373136	2.086754	0.070351
H	1.407602	0.939576	0.963646

H	0.915683	-2.985901	-0.833933
H	0.373901	-1.582973	-1.672851
H	0.634000	2.213532	-1.778663
H	0.359636	2.985901	-0.235722
H	-1.575146	2.125911	-1.049157
H	-0.021115	-1.123082	1.239076
H	-0.581079	-2.743260	0.861610
H	-2.341990	-1.975534	-0.238415
H	-2.072104	1.975217	1.119756
H	-0.625530	1.029963	1.437738
H	-2.470275	-0.527169	1.809148
H	-3.337810	0.024509	0.375478

Cu(L233)$^{2+}$(VI)

N	2.273552	-0.213831	-0.693304
C	2.383817	-1.622598	-0.180508
C	2.389638	0.900353	0.346423
Cu	0.409170	0.084281	-1.191907
C	1.502015	2.148121	0.058166
N	-0.105295	-1.670537	-0.388611
C	1.065860	-2.044289	0.482751
N	-0.905293	1.373350	-0.570340
C	-0.008533	2.099811	0.435371
C	-2.200073	0.826673	-0.010022
C	-1.446200	-1.640727	0.292020
C	-2.437537	-0.654654	-0.353681
H	2.982662	-0.067040	-1.412801
H	3.209454	-1.722665	0.530528
H	2.606696	-2.258545	-1.041123
H	3.436015	1.212046	0.391095
H	2.134909	0.475545	1.319735
H	1.641589	2.494901	-0.976434
H	1.926221	2.953762	0.666930
H	-0.155871	-2.310365	-1.187853
H	0.925274	-1.539596	1.440779
H	1.063956	-3.121738	0.675351
H	-1.137005	2.031044	-1.317867
H	-0.380386	3.121738	0.548078
H	-0.135343	1.597236	1.396376
H	-3.026409	1.421391	-0.406026
H	-2.188825	0.967540	1.072975
H	-1.280776	-1.390205	1.342242
H	-1.862732	-2.653176	0.254096
H	-2.475644	-0.799152	-1.440779
H	-3.436015	-0.913306	0.012969

Cu(L233H)$^{3+}$(VII)

N	0.812191	1.385298	0.720418
C	-0.603558	1.936564	0.639401
C	1.605394	1.387588	-0.577022
Cu	1.228729	-0.294606	1.717234
C	2.839793	0.474293	-0.514343

C	-1.660435	1.260795	-0.258618
N	1.485231	-1.574744	0.231336
N	-2.560754	0.186639	0.378457
C	2.563216	-1.042821	-0.689860
C	0.153747	-1.812366	-0.424234
C	-2.351717	-1.304211	0.065818
C	-1.029605	-1.905214	0.575254
H	1.295965	2.050539	1.340886
H	-0.493584	2.953792	0.242039
H	-0.969249	2.057250	1.664291
H	1.935038	2.420273	-0.749316
H	0.941652	1.118477	-1.399518
H	3.412293	0.657790	0.407533
H	3.518629	0.762031	-1.324331
H	-1.264960	0.848701	-1.186601
H	-2.345412	2.061390	-0.547978
H	1.811963	-2.442083	0.679790
H	-3.518629	0.392790	0.060954
H	-2.605783	0.316755	1.396931
H	3.483765	-1.593406	-0.482304
H	2.254874	-1.254728	-1.717234
H	0.232905	-2.742374	-1.000264
H	0.017037	-1.009282	-1.147790
H	-2.471852	-1.416290	-1.014438
H	-3.196193	-1.804674	0.546050
H	-0.781793	-1.450096	1.552008
H	-1.228108	-2.953792	0.814311

Cu(L233H)$^{3+}$(VIII)

N	2.263314	1.278991	-0.327091
C	2.222125	0.649869	1.051625
C	1.278468	2.383181	-0.688298
Cu	2.156502	-0.323966	-1.506499
C	-0.081514	1.940581	-1.285367
N	1.288620	-1.388566	-0.055181
C	1.159856	-0.443728	1.119485
C	-1.270357	1.838828	-0.297294
C	0.043778	-2.177764	-0.416782
N	-2.335565	0.829931	-0.724153
C	-1.112462	-1.460761	-1.152875
C	-2.156306	-0.643917	-0.331825
H	3.199729	1.686742	-0.442786
H	2.037950	1.423136	1.805133
H	3.219562	0.242580	1.242209
H	1.796179	2.998715	-1.426397
H	1.149104	3.002284	0.208332
H	0.051477	1.002229	-1.837350
H	-0.339347	2.678944	-2.049948
H	2.009274	-2.087036	0.175059
H	0.158138	-0.025767	1.092495
H	1.261187	-1.012429	2.049948
H	-1.775534	2.805210	-0.231802
H	-0.984885	1.563935	0.718139

H	-0.314546	-2.633764	0.517499
H	0.387070	-3.002284	-1.047500
H	-3.219562	1.129285	-0.289172
H	-2.512577	0.904529	-1.734947
H	-0.737129	-0.894761	-2.013119
H	-1.667583	-2.284604	-1.611617
H	-3.145279	-1.082793	-0.478335
H	-1.969135	-0.648698	0.743320

$Cu(L333)^{2+}$(IX)

N	0.302525	-2.079060	-0.006694
C	0.298954	-2.100750	1.502326
C	1.694450	-2.096737	-0.589681
Cu	-0.816407	-0.606843	-0.750371
C	-1.007083	-1.647790	2.174497
C	1.812574	-1.639810	-2.052551
N	-1.847966	0.191134	0.688819
N	0.114768	0.196791	-2.253446
C	-1.306503	-0.144350	2.047938
C	1.578174	-0.136178	-2.276512
C	-0.233090	1.659331	-1.974617
C	-1.726747	1.655015	0.264357
C	-0.407246	2.032178	-0.472374
H	-0.197044	-2.909388	-0.341520
H	1.124943	-1.466840	1.831890
H	0.527327	-3.126427	1.814295
H	2.072079	-3.121953	-0.501262
H	2.314841	-1.463309	0.047969
H	-0.898782	-1.878176	3.238923
H	-1.861247	-2.243798	1.830682
H	1.168027	-2.235211	-2.710646
H	2.837321	-1.867675	-2.362037
H	-2.837321	-0.063591	0.675881
H	-0.276798	-0.056199	-3.162593
H	-0.400436	0.446619	2.207106
H	-2.034689	0.161561	2.805156
H	1.997030	0.172913	-3.238923
H	2.072210	0.453629	-1.499599
H	-1.152166	1.877949	-2.524545
H	0.558872	2.282745	-2.399571
H	-1.816073	2.275916	1.160426
H	-2.587875	1.873756	-0.372453
H	-0.371595	3.126427	-0.446484
H	0.467067	1.714573	0.110293

$Cu(L333H)^{3+}$(X)

N	-2.316088	-1.360672	-1.726772
C	-2.323160	-1.363929	-0.197673
C	-0.975801	-1.341147	-2.483261
C	-2.154420	0.053306	0.414652
C	-0.076761	-0.098668	-2.285883
C	-1.248083	0.073108	1.673171

C	0.924074	-0.218382	-1.110693
N	-0.458826	1.353893	1.830366
N	1.422584	1.102387	-0.588889
Cu	-0.011845	2.266344	0.121494
C	2.451875	1.016135	0.520090
C	0.847089	1.220778	2.581841
C	1.937819	0.421842	1.843259
H	-2.787625	-2.225195	-2.028410
H	-2.920613	-0.606547	-2.077286
H	-1.535459	-2.055926	0.106414
H	-3.277050	-1.802949	0.101343
H	-1.258386	-1.419211	-3.535431
H	-0.461164	-2.266344	-2.212411
H	-3.136568	0.474239	0.644815
H	-1.717272	0.710578	-0.347870
H	-0.694387	0.806717	-2.217287
H	0.483940	0.016063	-3.218393
H	-0.527612	-0.743875	1.653092
H	-1.845304	-0.049599	2.583581
H	1.803785	-0.788820	-1.433192
H	0.498440	-0.753579	-0.263632
H	-1.040245	2.043111	2.327273
H	1.845108	1.630860	-1.365374
H	2.853512	2.024928	0.658105
H	3.277050	0.389483	0.154819
H	0.632665	0.717914	3.535431
H	1.181231	2.234854	2.822374
H	2.800151	0.398410	2.518349
H	1.654580	-0.626933	1.722796

B3LYP/LanL2DZ
$Zn(L222)^{2+}$(I)

N	0.529021	-0.753428	1.769357
C	0.529021	0.775816	1.769357
C	-0.861920	-1.386888	1.769357
Zn	1.180304	-1.267177	-0.120371
C	1.450687	1.387096	0.679871
N	1.274730	0.714987	-0.681596
N	-0.762506	-1.413970	-0.798708
C	-1.620679	-1.141788	0.438104
C	-0.070032	0.989292	-1.357741
C	-0.788932	-0.299458	-1.843325
H	1.045028	-1.098885	2.584440
H	0.863418	1.142744	2.744961
H	-0.502345	1.115817	1.642583
H	-1.462188	-0.990230	2.596503
H	-0.723871	-2.460548	1.943695
H	2.505312	1.273545	0.957533
H	1.241189	2.460548	0.603788
H	2.037361	1.021036	-1.294624
H	-1.065882	-2.286399	-1.243243
H	-1.981601	-0.111256	0.379749

H	-2.505312	-1.786308	0.422025
H	0.083127	1.640374	-2.224294
H	-0.696572	1.544715	-0.654004
H	-1.823657	-0.047157	-2.103151
H	-0.307276	-0.695626	-2.744961

Zn(L222H)$^{3+}$(II)

N	1.069319	-0.677413	1.750495
C	1.069319	0.860568	1.750495
C	-0.320058	-1.357407	1.750495
Zn	2.386417	-0.926384	0.195864
C	0.955240	1.501485	0.322465
N	1.479661	0.608809	-0.823649
C	-1.425362	-0.750831	0.864791
N	-1.517816	-1.233748	-0.606772
C	0.413313	0.120437	-1.821367
C	-0.280793	-1.228160	-1.527884
H	1.502473	-0.979347	2.637183
H	2.006943	1.170103	2.229814
H	0.258377	1.237967	2.383574
H	-0.694195	-1.267168	2.779434
H	-0.177212	-2.429994	1.571462
H	1.535756	2.429994	0.321969
H	-0.073801	1.781209	0.087262
H	2.138358	1.176054	-1.377312
H	-1.410352	0.339387	0.848552
H	-2.386417	-1.039661	1.308030
H	-2.264601	-0.674340	-1.057629
H	-1.876859	-2.205598	-0.602224
H	0.930819	-0.014160	-2.779434
H	-0.312822	0.928852	-1.977259
H	-0.643235	-1.619732	-2.487387
H	0.403072	-1.998097	-1.139366

Zn(L223)$^{2+}$(III)

N	0.509459	-0.208924	-1.868710
C	0.509459	1.336802	-1.868710
C	-0.898332	-0.821921	-1.868710
Zn	1.277207	-0.888375	-0.092575
C	0.942056	1.994930	-0.534665
N	0.729155	0.356776	1.428101
C	-0.972185	-2.188024	-1.145005
N	-0.350566	-2.121796	0.245942
C	0.158328	1.615218	0.748890
C	-1.167414	-1.346514	1.277797
C	-0.281556	-0.477747	2.209042
H	0.995438	-0.523303	-2.715937
H	-0.493558	1.672412	-2.154023
H	1.195502	1.666430	-2.655408
H	-1.246204	-0.947601	-2.899632
H	-1.566763	-0.099158	-1.392548

H	0.831578	3.076480	-0.686576
H	2.022912	1.849770	-0.365018
H	1.470158	0.653230	2.073333
H	-0.432891	-2.960866	-1.704911
H	-2.022912	-2.495670	-1.084106
H	-0.189452	-3.076480	0.582322
H	-0.899363	1.433020	0.532124
H	0.200809	2.437977	1.469892
H	-1.743694	-2.043192	1.895435
H	-1.890604	-0.724883	0.741731
H	-0.927818	0.172522	2.810097
H	0.287293	-1.111005	2.899632

$Zn(L223H)^{3+}$(IV)

N	0.717016	-0.523665	-1.804843
C	0.717016	1.046902	-1.804843
C	-0.663666	-1.205362	-1.804843
Zn	1.926155	-0.909237	-0.219406
C	1.780949	1.661695	-0.858479
N	1.358869	0.285230	1.319367
C	-1.114163	-1.891267	-0.493682
N	-1.903626	-1.043128	0.526667
C	1.494332	1.701443	0.664205
C	0.001250	0.025658	2.010122
C	-1.275107	0.221392	1.160420
H	1.160706	-0.804132	-2.692055
H	-0.289999	1.387003	-1.548760
H	0.913336	1.369517	-2.832086
H	-0.617069	-2.004520	-2.553885
H	-1.410171	-0.490907	-2.173774
H	1.916159	2.708222	-1.169617
H	2.787537	1.232166	-1.067314
H	2.041799	0.247914	2.092011
H	-0.287688	-2.367207	0.053471
H	-1.795313	-2.708222	-0.764072
H	-2.787537	-0.741715	0.078072
H	-2.193099	-1.680525	1.290275
H	0.585489	2.270588	0.880609
H	2.319382	2.215311	1.168378
H	-0.060059	0.750181	2.832086
H	0.043901	-0.964574	2.481751
H	-2.058101	0.611878	1.821166
H	-1.150568	0.952037	0.359453

$Zn(L223H)^{3+}$(V)

N	0.919513	-0.328993	-2.040384
C	0.919513	1.215041	-2.040384
C	-0.470002	-1.002424	-2.040384
Zn	1.721293	-1.007953	-0.297345
C	0.770815	1.860759	-0.637386
C	-0.618281	-2.119689	-0.968034

N	-0.086221	-1.697277	0.421973
C	-0.685892	2.007092	-0.106463
C	-1.070064	-0.827751	1.237073
N	-0.839604	1.776197	1.412892
C	-0.469288	0.386371	1.993863
H	1.420308	-0.626039	-2.890496
H	0.137884	1.562693	-2.726949
H	1.880955	1.520210	-2.467280
H	-0.645872	-1.453977	-3.022775
H	-1.224431	-0.224590	-1.912909
H	1.225226	2.857699	-0.696781
H	1.420581	1.331501	0.096629
H	-0.066395	-3.023576	-1.261538
H	-1.674149	-2.404027	-0.893734
H	0.054462	-2.561826	0.964882
H	-1.389912	1.327788	-0.587519
H	-1.050655	3.023576	-0.291508
H	-1.524078	-1.493185	1.979412
H	-1.880955	-0.525761	0.567096
H	-0.290422	2.487885	1.926939
H	-1.828245	1.972273	1.650344
H	0.622363	0.341556	2.075242
H	-0.845997	0.400502	3.022775

$Zn(L233)^{2+}$(VI)

N	0.373230	-0.242834	-2.344009
C	0.373230	1.284589	-2.344009
C	-1.027150	-0.883254	-2.344009
Zn	1.262949	-0.685005	-0.553799
C	-1.125557	-2.204259	-1.539535
N	1.070357	1.248819	0.104255
C	0.119299	1.853548	-0.926034
N	0.241868	-1.939653	0.656821
C	-1.152523	-2.071488	0.005323
C	0.199418	-1.375543	2.096364
C	0.529189	1.192912	1.544822
C	1.000778	-0.068327	2.312054
H	0.868130	-0.564527	-3.183206
H	-0.396061	1.665460	-3.025706
H	1.346709	1.613687	-2.726294
H	-1.315621	-1.065789	-3.384614
H	-1.729738	-0.146619	-1.938621
H	-0.355446	-2.921707	-1.863887
H	-2.077790	-2.667920	-1.828252
H	1.938572	1.796705	0.113926
H	-0.902413	1.632089	-0.600561
H	0.220377	2.943768	-0.953797
H	0.640205	-2.885018	0.704144
H	-1.646841	-2.943768	0.446713
H	-1.730742	-1.187826	0.298769
H	0.595316	-2.143485	2.768403
H	-0.852018	-1.223213	2.362633

H	-0.564657	1.229120	1.494314
H	0.857225	2.092764	2.074741
H	2.077790	-0.237982	2.139922
H	0.926073	0.155219	3.384614

Zn(L233H)$^{3+}$(VII)

N	0.619129	-0.061835	-1.848450
C	0.619129	1.491728	-1.848450
C	-0.778564	-0.765812	-1.848450
Zn	1.661150	-1.162975	-0.493299
C	-0.761850	-2.185207	-1.216530
C	-0.353843	2.293042	-0.958293
N	0.625579	-2.006867	1.000916
N	-0.069823	2.421903	0.561614
C	-0.758712	-2.301217	0.332836
C	0.620738	-1.088475	2.238020
C	-0.405259	1.184456	1.433801
C	0.853229	0.409769	1.909338
H	1.037190	-0.285754	-2.766678
H	0.346195	1.794983	-2.868675
H	1.656359	1.816850	-1.701752
H	-1.117186	-0.827805	-2.888016
H	-1.483478	-0.127634	-1.312521
H	0.021321	-2.825053	-1.670942
H	-1.689030	-2.672340	-1.551792
H	-1.394305	1.969530	-1.047077
H	-0.311566	3.319793	-1.344375
H	1.002922	-2.913410	1.312648
H	0.902650	2.731331	0.722084
H	-0.662725	3.205372	0.888036
H	-1.042711	-3.319793	0.614792
H	-1.495270	-1.627037	0.779217
H	1.432179	-1.431987	2.888016
H	-0.316176	-1.240815	2.786963
H	-1.090787	0.576539	0.841525
H	-0.961291	1.544984	2.305068
H	1.689030	0.511178	1.179027
H	1.246143	0.886252	2.816614

Zn(L233H)$^{3+}$(VIII)

N	1.011098	-0.713800	2.301561
C	1.011098	0.829497	2.301561
C	-0.357463	-1.417051	2.301561
Zn	1.767640	-1.613102	0.626395
C	1.025591	1.500770	0.895917
N	-0.057807	-2.084223	-0.178911
C	-0.998572	-1.505994	0.891445
C	-0.336081	2.091575	0.431159

C	-0.400672	-1.656259	-1.627826
N	-0.486129	2.186848	-1.104616
C	-0.000477	-0.226013	-2.079872
C	-1.027818	0.931736	-1.844249
H	1.494424	-0.998700	3.166063
H	1.915553	1.122508	2.843518
H	0.156294	1.163960	2.902826
H	-1.044882	-0.884430	2.968713
H	-0.207788	-2.417125	2.729499
H	1.417432	0.790029	0.146915
H	1.762856	2.312138	0.920178
H	-0.172036	-3.110576	-0.174298
H	-1.308870	-0.520826	0.547426
H	-1.894907	-2.132965	0.958300
H	-0.439891	3.110576	0.819340
H	-1.201636	1.525042	0.783985
H	-1.476867	-1.822415	-1.766895
H	0.117356	-2.375980	-2.270691
H	-1.165052	2.944751	-1.293702
H	0.399728	2.496814	-1.536729
H	0.129429	-0.308505	-3.166063
H	1.005459	0.037818	-1.718810
H	-1.376888	1.305136	-2.812357
H	-1.915553	0.616296	-1.288292

$Zn(L333)^{2+}$(IX)

N	-0.210005	-0.097913	-2.245448
C	-0.210005	1.444355	-2.245448
C	-1.625636	-0.708933	-2.245448
Zn	0.821872	-0.788425	-0.637224
C	1.027987	2.086106	-1.574241
C	-1.710147	-2.128024	-1.633656
N	1.678823	0.665543	0.479688
N	-0.156459	-2.202038	0.429839
C	1.093471	1.993691	-0.028001
C	-1.604146	-2.215710	-0.089762
C	-0.047647	-1.844605	1.921237
C	1.372558	0.388917	1.960237
C	0.018752	-0.323084	2.210427
H	0.246331	-0.398470	-3.116858
H	-1.118034	1.767389	-1.725020
H	-0.288827	1.790546	-3.281774
H	-1.994306	-0.727890	-3.276949
H	-2.271179	-0.026464	-1.681774
H	0.991946	3.153359	-1.828460
H	1.962704	1.721080	-2.029009
H	-0.996393	-2.814584	-2.116073
H	-2.699679	-2.518066	-1.905196
H	2.699679	0.730118	0.380659
H	0.213751	-3.153359	0.311243
H	0.092693	2.101506	0.406419

H	1.709842	2.807490	0.370078
H	-2.080403	-3.136329	0.265722
H	-2.130800	-1.376427	0.379269
H	0.849055	-2.341357	2.310191
H	-0.911823	-2.277963	2.438056
H	1.386491	1.346128	2.494486
H	2.195743	-0.217985	2.355247
H	-0.190652	-0.208267	3.281774
H	-0.805459	0.210639	1.710578

$Zn(L333H)^{3+}$(X)

N	2.578868	-0.945416	-1.312401
C	2.578868	0.615085	-1.312401
C	1.220629	-1.684590	-1.312401
C	1.958906	1.315761	-0.072687
C	0.626791	-1.859759	0.116430
C	0.435743	1.600831	-0.203662
C	-0.932034	-1.890045	0.135592
N	-0.289172	1.785844	1.133442
N	-1.540086	-1.275934	1.412459
Zn	-0.325514	0.103160	2.241820
C	-2.835820	-0.442007	1.140418
C	-1.822524	2.044367	0.948259
C	-2.622766	0.865412	0.334710
H	3.168892	-1.288595	-0.537500
H	3.073866	-1.219984	-2.179116
H	2.084416	0.917824	-2.241820
H	3.636140	0.887841	-1.396392
H	1.393079	-2.660994	-1.776738
H	0.564442	-1.114700	-1.976560
H	2.492776	2.267949	0.034514
H	2.205049	0.755552	0.844812
H	0.986895	-1.016952	0.736120
H	1.033048	-2.766213	0.580334
H	-0.079173	0.797155	-0.734643
H	0.282724	2.517026	-0.788464
H	-1.297392	-2.918765	0.048880
H	-1.338707	-1.330974	-0.711287
H	0.102417	2.615824	1.603181
H	-1.809064	-2.044428	2.043706
H	-3.286820	-0.241731	2.121567
H	-3.531067	-1.087724	0.591792
H	-1.928101	2.918765	0.295598
H	-2.213385	2.329524	1.934407
H	-3.636140	1.265756	0.184900
H	-2.275489	0.647213	-0.681997

B3LYP/DZVP2
$Zn(L222)^{2+}$(I)

N	0.505764	-0.748056	1.756227
C	0.505764	0.768296	1.756227
C	-0.867715	-1.381147	1.756227
Zn	1.151402	-1.244945	-0.099761
C	1.420898	1.377895	0.667379
N	1.259056	0.695947	-0.672840
N	-0.742019	-1.433451	-0.798729
C	-1.613857	-1.178001	0.415566
C	-0.066683	0.955632	-1.361918
C	-0.769822	-0.337718	-1.840749
H	1.018564	-1.092607	2.567662
H	0.841041	1.133461	2.728889
H	-0.524186	1.105308	1.631279
H	-1.478078	-0.969784	2.565204
H	-0.721749	-2.446230	1.955655
H	2.472465	1.272676	0.947850
H	1.202814	2.446230	0.581439
H	2.024814	0.991363	-1.278173
H	-1.019794	-2.307879	-1.244034
H	-2.008372	-0.163813	0.339441
H	-2.472465	-1.851971	0.396341
H	0.093179	1.598948	-2.229311
H	-0.702657	1.511282	-0.671297
H	-1.800991	-0.097129	-2.114701
H	-0.272583	-0.737121	-2.728889

$Zn(L222H)^{3+}$(II)

N	1.066738	-0.669366	1.754160
C	1.066738	0.852333	1.754160
C	-0.300202	-1.353704	1.754160
Zn	2.344362	-0.895056	0.212696
C	0.952664	1.494692	0.329387
N	1.502033	0.628179	-0.804911
C	-1.383912	-0.815857	0.810127
N	-1.399069	-1.313451	-0.642009
C	0.478579	0.130271	-1.816142
C	-0.169277	-1.240082	-1.546052
H	1.510070	-0.968097	2.630101
H	2.006148	1.156283	2.225870
H	0.258090	1.229871	2.386663
H	-0.705155	-1.206179	2.761911
H	-0.141935	-2.430490	1.642393
H	1.515347	2.430490	0.341176
H	-0.077461	1.750001	0.083932
H	2.173132	1.195348	-1.332641
H	-1.423935	0.271699	0.780053
H	-2.344362	-1.145847	1.217914
H	-2.174075	-0.820448	-1.111440
H	-1.699117	-2.299912	-0.640277
H	1.016510	0.015184	-2.761911
H	-0.268187	0.914776	-1.977136
H	-0.508425	-1.634033	-2.509808
H	0.545390	-1.986089	-1.168058

$Zn(L223)^{2+}$(III)

N	0.477571	-0.213558	-1.848425
C	0.477571	1.318353	-1.848425
C	-0.913802	-0.828534	-1.848425
Zn	1.227988	-0.868364	-0.106281
C	0.954247	1.972197	-0.535135
N	0.761784	0.340154	1.414293
C	-0.985215	-2.181304	-1.111102
N	-0.349858	-2.104404	0.255270
C	0.215549	1.612102	0.772951
C	-1.137932	-1.336087	1.293621
C	-0.231322	-0.478100	2.206003
H	0.963325	-0.527388	-2.688880
H	-0.530952	1.651532	-2.103051
H	1.137502	1.644704	-2.653956
H	-1.257957	-0.965105	-2.876224
H	-1.584187	-0.105016	-1.381940
H	0.856557	3.052241	-0.686649
H	2.033675	1.807921	-0.400682
H	1.524844	0.603634	2.038649
H	-0.451891	-2.957225	-1.666770
H	-2.033675	-2.484945	-1.038232
H	-0.177593	-3.052241	0.589525
H	-0.854284	1.470905	0.603528
H	0.320337	2.424309	1.495330
H	-1.707375	-2.028438	1.917586
H	-1.863625	-0.709143	0.772607
H	-0.856865	0.172582	2.823432
H	0.348395	-1.118288	2.876224

$Zn(L223H)^{3+}$(IV)

N	0.704109	-0.481152	-1.806155
C	0.704109	1.073774	-1.806155
C	-0.650818	-1.178571	-1.806155
Zn	1.828413	-0.822424	-0.211461
C	1.751824	1.679309	-0.842699
N	1.333761	0.321968	1.326207
C	-1.061650	-1.891063	-0.502546
N	-1.839694	-1.094834	0.546343
C	1.450297	1.725831	0.672315
C	0.008151	0.048272	2.032047
C	-1.276570	0.176055	1.192278
H	1.168077	-0.767104	-2.673589
H	-0.306001	1.411202	-1.569995
H	0.922807	1.394216	-2.826516
H	-0.594026	-1.967389	-2.560649
H	-1.414009	-0.476200	-2.154822
H	1.921339	2.716696	-1.157007
H	2.747915	1.219511	-1.026149

H	2.035465	0.279723	2.073112
H	-0.211375	-2.359411	0.011051
H	-1.728543	-2.716696	-0.770581
H	-2.747915	-0.832158	0.134806
H	-2.089698	-1.757169	1.295804
H	0.531246	2.277087	0.878276
H	2.263409	2.249505	1.178943
H	-0.071922	0.797315	2.826516
H	0.084261	-0.921402	2.534202
H	-2.073081	0.508564	1.863912
H	-1.202514	0.926173	0.405488

$Zn(L223H)^{3+}$(V)

N	0.921868	-0.298890	-2.047405
C	0.921868	1.226256	-2.047405
C	-0.445173	-0.983406	-2.047405
Zn	1.669496	-0.922453	-0.302362
C	0.788257	1.850448	-0.640702
C	-0.587401	-2.095693	-0.972626
N	-0.062790	-1.684562	0.404848
C	-0.654567	1.976389	-0.084086
C	-1.027581	-0.860066	1.261339
N	-0.790104	1.735330	1.416452
C	-0.429301	0.361256	1.997254
H	1.438925	-0.606072	-2.877156
H	0.137014	1.578218	-2.724109
H	1.880051	1.530302	-2.474397
H	-0.609686	-1.445295	-3.023975
H	-1.207715	-0.215485	-1.928288
H	1.242731	2.845547	-0.679950
H	1.453948	1.310325	0.071177
H	-0.022002	-2.987305	-1.264468
H	-1.638290	-2.390519	-0.901540
H	0.116862	-2.551690	0.919441
H	-1.359260	1.295910	-0.557549
H	-1.032371	2.987305	-0.256576
H	-1.417164	-1.541153	2.021336
H	-1.880051	-0.581940	0.637849
H	-0.246545	2.442272	1.933565
H	-1.769209	1.940616	1.663319
H	0.659857	0.311395	2.078156
H	-0.804146	0.385115	3.023975

$Zn(L233)^{2+}$(VI)

N	0.316531	-0.116989	-2.317371
C	0.316531	1.394160	-2.317371
C	-1.059250	-0.772496	-2.317371
Zn	1.156772	-0.561985	-0.554988
C	-1.104786	-2.134406	-1.590972
N	1.052891	1.334268	0.100564

C	0.105715	1.962267	-0.896544
N	0.218065	-1.835751	0.616096
C	-1.135554	-2.099565	-0.048010
C	0.122403	-1.259962	2.035079
C	0.567434	1.296822	1.545798
C	0.973135	0.002123	2.282343
H	0.816851	-0.435363	-3.147377
H	-0.465333	1.779193	-2.977892
H	1.280356	1.716404	-2.720512
H	-1.374282	-0.897812	-3.355835
H	-1.759391	-0.073830	-1.851659
H	-0.312650	-2.800176	-1.957808
H	-2.038943	-2.615193	-1.899793
H	1.937079	1.844042	0.077195
H	-0.910813	1.759899	-0.551480
H	0.228870	3.047716	-0.921080
H	0.697186	-2.734856	0.681016
H	-1.519128	-3.047716	0.336084
H	-1.815029	-1.314168	0.292335
H	0.433961	-2.038748	2.733419
H	-0.931135	-1.051724	2.232560
H	-0.519323	1.409875	1.533401
H	0.974367	2.162823	2.071436
H	2.038943	-0.211615	2.114003
H	0.898607	0.207323	3.355835

$Zn(L233H)^{3+}$(VII)

N	0.533381	-0.022242	-1.812406
C	0.533381	1.511049	-1.812406
C	-0.847601	-0.728615	-1.812406
Zn	1.519594	-1.099994	-0.481261
C	-0.812436	-2.153145	-1.205832
C	-0.355615	2.304507	-0.841949
N	0.603587	-2.027483	0.976232
N	0.011896	2.376675	0.646535
C	-0.780650	-2.310820	0.335432
C	0.644559	-1.165078	2.233142
C	-0.329604	1.154699	1.511428
C	0.905485	0.330576	1.943965
H	0.956885	-0.250391	-2.719600
H	0.174475	1.817946	-2.801385
H	1.577059	1.832881	-1.751712
H	-1.189943	-0.777641	-2.848556
H	-1.548617	-0.100689	-1.263689
H	-0.021320	-2.763869	-1.677366
H	-1.732447	-2.646171	-1.542074
H	-1.406617	2.014637	-0.879447
H	-0.303886	3.338178	-1.198755
H	1.011167	-2.934028	1.223414
H	0.996179	2.650816	0.765088
H	-0.518281	3.177218	1.019197
H	-1.046819	-3.338178	0.591014
H	-1.509687	-1.658174	0.818344

H	1.466436	-1.544818	2.843229
H	-0.278412	-1.317905	2.799902
H	-1.056775	0.581091	0.938265
H	-0.846138	1.527800	2.397877
H	1.732447	0.421842	1.204605
H	1.334449	0.774039	2.848556

$Zn(L233H)^{3+}$(VIII)

N	0.997964	-0.662500	2.307453
C	0.997964	0.862794	2.307453
C	-0.341697	-1.387691	2.307453
Zn	1.724391	-1.506089	0.640945
C	1.007223	1.521610	0.904336
N	-0.032604	-2.055985	-0.160856
C	-0.981268	-1.519112	0.902305
C	-0.355362	2.066608	0.410807
C	-0.380209	-1.662206	-1.598690
N	-0.477214	2.155736	-1.109500
C	0.018527	-0.247616	-2.075163
C	-0.990530	0.924749	-1.871293
H	1.491287	-0.953816	3.156985
H	1.908122	1.151018	2.836019
H	0.152243	1.200763	2.914383
H	-1.043256	-0.867594	2.966131
H	-0.162238	-2.376304	2.741960
H	1.434893	0.818416	0.169677
H	1.721550	2.349556	0.929982
H	-0.091111	-3.080639	-0.140799
H	-1.341923	-0.555591	0.551034
H	-1.843890	-2.186287	0.982795
H	-0.496507	3.080639	0.792148
H	-1.210591	1.479795	0.746696
H	-1.452534	-1.838798	-1.731342
H	0.142282	-2.388331	-2.225158
H	-1.150509	2.908495	-1.310165
H	0.403889	2.487364	-1.524386
H	0.141312	-0.353923	-3.156985
H	1.028159	0.013075	-1.730669
H	-1.285997	1.314961	-2.847201
H	-1.908122	0.621814	-1.363695

$Zn(L333)^{3+}$(IX)

N	-0.244210	-0.068099	-2.234824
C	-0.244210	1.457257	-2.234824
C	-1.638806	-0.684809	-2.234824
Zn	0.780926	-0.747552	-0.677965
C	1.001760	2.095235	-1.591284
C	-1.705249	-2.107046	-1.646045
N	1.693513	0.640364	0.398132
N	-0.104197	-2.185478	0.353883
C	1.123392	1.974738	-0.057142
C	-1.550897	-2.226463	-0.115027

C	0.062402	-1.890193	1.837117
C	1.474190	0.337159	1.872389
C	0.147509	-0.388137	2.182097
H	0.213019	-0.366632	-3.098933
H	-1.139474	1.775732	-1.695777
H	-0.347264	1.803964	-3.265807
H	-2.016319	-0.689110	-3.260272
H	-2.281498	-0.016955	-1.656126
H	0.944190	3.164451	-1.819985
H	1.921787	1.751810	-2.082661
H	-1.011041	-2.783602	-2.161858
H	-2.701958	-2.488574	-1.890821
H	2.701958	0.680966	0.241006
H	0.288869	-3.112190	0.181002
H	0.144881	2.093566	0.416571
H	1.769044	2.767005	0.330563
H	-1.991223	-3.164451	0.232980
H	-2.081934	-1.413626	0.388145
H	0.971241	-2.402134	2.164385
H	-0.777447	-2.342418	2.371453
H	1.514412	1.280057	2.424470
H	2.320178	-0.271018	2.203100
H	0.008999	-0.317471	3.265807
H	-0.705886	0.160836	1.761343

$Zn(L333H)^{3+}$(X)

N	2.572787	-0.840916	-1.245186
C	2.572787	0.701751	-1.245186
C	1.244621	-1.599472	-1.245186
C	1.936814	1.409701	-0.025253
C	0.665593	-1.802001	0.178334
C	0.426729	1.721382	-0.179473
C	-0.885115	-1.879624	0.219882
N	-0.316286	1.859879	1.135155
N	-1.485752	-1.237727	1.467832
Zn	-0.301058	0.176530	2.144409
C	-2.786125	-0.443171	1.200667
C	-1.841909	2.061165	0.952390
C	-2.608703	0.849617	0.372259
H	3.174644	-1.184502	-0.485728
H	3.071429	-1.111314	-2.104701
H	2.100285	1.002608	-2.183419
H	3.630101	0.967915	-1.310028
H	1.437117	-2.564319	-1.719533
H	0.573894	-1.039275	-1.899117
H	2.483786	2.349518	0.093956
H	2.152892	0.849597	0.895449
H	1.009175	-0.953470	0.796291
H	1.109058	-2.687659	0.642499
H	-0.088144	0.945547	-0.747278
H	0.292165	2.656704	-0.732208
H	-1.223200	-2.917532	0.179323
H	-1.317779	-1.364448	-0.638326

H	0.040813	2.682582	1.632303
H	-1.716096	-1.975498	2.140117
H	-3.220194	-0.233315	2.183419
H	-3.476328	-1.110986	0.677563
H	-1.977302	2.917532	0.285659
H	-2.230188	2.350211	1.934157
H	-3.630101	1.220307	0.223113
H	-2.265517	0.621594	-0.641142

B3LYP/LanL2DZ
$Cd(L222)^{2+}$(I)

N	0.572898	-0.768064	-1.772540
C	0.572898	0.754003	-1.772540
C	-0.812355	-1.400490	-1.772540
Cd	1.360066	-1.427639	0.271789
C	1.443495	1.402245	-0.663276
N	1.218918	0.810795	0.721758
N	-0.861253	-1.379031	0.815468
C	-1.624912	-1.131989	-0.477813
C	-0.168388	1.056187	1.297502
C	-0.896664	-0.218857	1.801115
H	1.085599	-1.114577	-2.589463
H	-0.463082	1.095301	-1.694535
H	0.947414	1.117800	-2.735473
H	-0.674759	-2.477810	-1.925447
H	-1.398687	-1.021662	-2.619626
H	1.224850	2.477810	-0.652947
H	2.509607	1.286989	-0.893551
H	1.929449	1.191739	1.354436
H	-1.231466	-2.212069	1.283724
H	-1.992857	-0.102215	-0.464130
H	-2.509607	-1.777166	-0.507233
H	-0.768308	1.564798	0.537609
H	-0.093523	1.745089	2.145809
H	-1.936251	0.055616	2.021743
H	-0.446870	-0.576023	2.735473

$Cd(L222H)^{3+}$(II)

C	1.585494	-1.035486	0.823843
C	1.585494	0.532996	0.823843
N	0.205158	-1.689217	0.823843
N	0.357333	1.200799	1.453102
C	-0.475993	-1.852641	-0.549058
Cd	-0.693061	-0.499867	2.574232
C	-0.556956	1.950090	0.477642
C	-0.319560	-0.719336	-1.580610
C	-1.684024	1.157721	-0.220414
N	-1.355987	0.433288	-1.541098
H	2.105073	-1.408534	1.716240
H	2.170363	-1.384242	-0.036248
H	1.699656	0.928033	-0.188673

H	2.471547	0.859321	1.379041
H	0.328935	-2.654001	1.165805
H	0.697472	1.910753	2.117096
H	-1.525184	-2.126163	-0.385830
H	-0.004478	-2.728841	-1.016455
H	0.071521	2.479763	-0.252079
H	-1.059521	2.728841	1.064685
H	-0.445375	-1.166492	-2.574232
H	0.672190	-0.266724	-1.570572
H	-2.471547	1.875558	-0.482873
H	-2.158965	0.411521	0.431403
H	-1.050982	1.137165	-2.237223
H	-2.253142	0.065568	-1.904829

Cd(L223)$^{2+}$(III)

N	0.600918	-0.233795	1.907341
C	0.600918	1.304556	1.907341
C	-0.798910	-0.845481	1.907341
Cd	1.520976	-0.947253	-0.050110
C	0.920711	1.981475	0.550771
N	0.533440	0.480271	-1.503915
C	-0.922380	-2.191567	1.156066
N	-0.443238	-2.110883	-0.284292
C	0.017554	1.660298	-0.671411
C	-1.320877	-1.267131	-1.195107
C	-0.534451	-0.363611	-2.179192
H	1.091768	-0.550841	2.750209
H	1.352385	1.631737	2.633713
H	-0.372577	1.644870	2.279755
H	-1.477409	-0.106425	1.473399
H	-1.128510	-1.003099	2.940952
H	1.979702	1.815007	0.279250
H	0.859400	3.061300	0.739966
H	1.157757	0.847591	-2.230770
H	-1.976037	-2.497956	1.191341
H	-0.338484	-2.975104	1.653849
H	-0.367946	-3.061300	-0.660132
H	-0.038389	2.537448	-1.325294
H	-1.006352	1.435204	-0.357218
H	-1.979702	-0.660678	-0.567601
H	-1.970547	-1.919569	-1.789407
H	-1.255913	0.280660	-2.698098
H	-0.032306	-0.971842	-2.940952

Cd(L223H)$^{3+}$(IV)

N	0.772263	-0.544004	1.796966
C	0.772263	1.015055	1.796966
C	-0.598844	-1.229953	1.796966
Cd	2.190284	-1.034707	0.090213
C	1.781951	1.664728	0.816969

N	1.271019	0.399728	-1.415021
C	-1.093770	-1.851285	0.470140
N	-1.944578	-0.964707	-0.461367
C	1.430453	1.764254	-0.687130
C	-0.126524	0.146839	-2.013493
C	-1.347772	0.319543	-1.082384
H	1.216014	-0.826680	2.682554
H	1.014562	1.336214	2.815437
H	-0.246284	1.358536	1.596089
H	-1.341368	-0.543409	2.225358
H	-0.527034	-2.066936	2.501559
H	2.796809	1.224308	0.959351
H	1.937882	2.698166	1.160661
H	1.888181	0.428469	-2.240590
H	-1.744756	-2.698166	0.720975
H	-0.279399	-2.265212	-0.139617
H	-2.796809	-0.680008	0.053778
H	-2.282959	-1.569559	-1.230711
H	2.231115	2.313137	-1.194941
H	0.515109	2.347060	-0.832515
H	-0.249338	0.886974	-2.815437
H	-0.115328	-0.832467	-2.508727
H	-1.168069	1.017578	-0.263912
H	-2.167056	0.738414	-1.678377

$Cd(L223H)^{3+}$(V)

N	0.952742	-0.353784	2.008918
C	0.952742	1.185670	2.008918
C	-0.428923	-1.020799	2.008918
Cd	1.961634	-1.154972	0.143270
C	0.741687	1.855556	0.626426
C	-0.632573	-2.121501	0.931009
N	-0.193820	-1.712657	-0.482344
C	-0.737223	2.017290	0.168357
C	-1.189103	-0.797074	-1.217228
N	-0.959117	1.808004	-1.345566
C	-0.597589	0.431480	-1.958807
H	1.451077	-0.647125	2.861132
H	1.929468	1.490891	2.399773
H	0.200425	1.528611	2.731536
H	-1.184643	-0.239413	1.915615
H	-0.592576	-1.492841	2.984431
H	1.344626	1.328277	-0.141740
H	1.200719	2.850124	0.684417
H	-1.693877	-2.399835	0.928337
H	-0.073898	-3.031750	1.192001
H	-0.125083	-2.576296	-1.038436
H	-1.090307	3.031750	0.384027
H	-1.420603	1.332941	0.670829
H	-1.961634	-0.498913	-0.501120
H	-1.694773	-1.422226	-1.961531
H	-1.958882	1.996436	-1.536616

H	-0.439003	2.532217	-1.871317
H	-0.981129	0.468165	-2.984431
H	0.492989	0.385950	-2.040936

Cd(L233)$^{2+}$(VI)

N	0.539568	-0.306844	2.398501
C	0.539568	1.215850	2.398501
C	-0.859573	-0.943394	2.398501
Cd	1.614009	-0.809576	0.461979
C	-1.068244	-2.119028	1.411062
N	1.149658	1.359118	-0.081700
C	0.195885	1.809315	1.013624
N	0.132892	-1.832140	-0.872051
C	-1.190611	-1.759027	-0.094953
C	0.084789	-1.130167	-2.239220
C	0.561287	1.383396	-1.500995
C	0.943223	0.152295	-2.362378
H	1.035152	-0.624631	3.238299
H	1.531019	1.548896	2.729690
H	-0.190590	1.591753	3.126245
H	-1.586794	-0.152131	2.184608
H	-1.064757	-1.296906	3.414935
H	-2.014183	-2.591145	1.706514
H	-0.309009	-2.902749	1.568231
H	1.975538	1.968017	-0.068388
H	0.192830	2.902749	1.094873
H	-0.813794	1.509166	0.715490
H	0.337809	-2.825517	-1.030403
H	-1.586014	-0.744425	-0.218283
H	-1.900995	-2.436964	-0.582388
H	0.433697	-1.845786	-2.991043
H	-0.963530	-0.907330	-2.470743
H	-0.527432	1.469298	-1.416555
H	0.912379	2.291802	-2.001723
H	0.870191	0.458140	-3.414935
H	2.014183	-0.086933	-2.222803

Cd(L233H)$^{3+}$(VII)

N	0.518838	-0.070114	1.914764
C	0.518838	1.482358	1.914764
C	-0.861923	-0.783183	1.914764
Cd	1.767966	-1.333603	0.479229
C	-0.862364	-2.187007	1.253089
C	-0.561576	2.290347	1.164479
N	0.317910	-1.980537	-1.093273
N	-0.450164	2.473797	-0.371485
C	-0.979668	-2.285872	-0.291724
C	0.214873	-0.951211	-2.227619
C	-0.808658	1.251612	-1.252443
C	0.442910	0.522650	-1.803361

H	0.943280	-0.296260	2.827740
H	1.525237	1.812755	1.631979
H	0.383822	1.788842	2.961496
H	-1.585530	-0.143560	1.407168
H	-1.189697	-0.873546	2.956417
H	-1.743998	-2.709654	1.652033
H	-0.028475	-2.815087	1.633778
H	-0.493571	3.306749	1.573143
H	-1.579882	1.944345	1.359077
H	0.608063	-2.863183	-1.537265
H	0.484695	2.835638	-0.620222
H	-1.111248	3.234633	-0.606769
H	-1.767966	-1.623095	-0.661414
H	-1.280620	-3.306749	-0.548481
H	0.981291	-1.222219	-2.961496
H	-0.755980	-1.073878	-2.725309
H	-1.449386	0.614683	-0.641684
H	-1.414380	1.622094	-2.085704
H	0.807126	1.061614	-2.687322
H	1.281584	0.580206	-1.077819

$Cd(L233H)^{3+}$(VIII)

N	1.083507	-0.774339	-2.290998
C	1.083507	0.762793	-2.290998
C	-0.278997	-1.467376	-2.290998
Cd	1.989446	-1.827965	-0.486409
C	1.055148	1.440703	-0.887457
N	-0.166987	-2.107276	0.223506
C	-0.981857	-1.487265	-0.910871
C	-0.298835	2.102630	-0.503955
C	-0.582849	-1.626147	1.629780
N	-0.529608	2.212601	1.022026
C	-0.162660	-0.193822	2.059168
C	-1.148704	0.979146	1.737156
H	1.569958	-1.063646	-3.151666
H	0.243634	1.096669	-2.915269
H	1.999675	1.059562	-2.810500
H	-0.130286	-2.486777	-2.672095
H	-0.945744	-0.961659	-3.001017
H	1.833674	2.212550	-0.868323
H	1.353738	0.706897	-0.122407
H	-0.343865	-3.123714	0.221854
H	-1.239898	-0.474780	-0.606876
H	-1.919764	-2.044906	-1.023437
H	-1.169401	1.574911	-0.902180
H	-0.332732	3.123714	-0.898747
H	-0.135316	-2.340392	2.328878
H	-1.672154	-1.748056	1.708302
H	-1.193503	2.992450	1.169011
H	0.341425	2.497214	1.498732
H	0.861311	0.029394	1.724153
H	-0.079798	-0.241138	3.151666

H	-1.999675	0.672961	1.122255
H	-1.559058	1.372158	2.672893

$Cd(L333)^{2+}$(IX)

N	-0.085912	-0.109970	2.249567
C	-0.085912	1.430678	2.249567
C	-1.493752	-0.732435	2.249567
Cd	1.070657	-0.888207	0.488332
C	1.049923	2.098975	1.435411
C	-1.605869	-2.119490	1.566834
N	1.536656	0.877830	-0.798641
N	-0.328476	-2.166719	-0.696658
C	0.898618	2.090867	-0.110312
C	-1.686780	-2.123488	0.016219
C	-0.384350	-1.644354	-2.137688
C	0.999336	0.628909	-2.212706
C	-0.368056	-0.100064	-2.284145
H	0.377708	-0.413039	3.114992
H	-0.032114	1.773958	3.288846
H	-1.053515	1.757249	1.854305
H	-2.161072	-0.026020	1.744895
H	-1.834298	-0.811109	3.288394
H	2.037742	1.711783	1.736125
H	1.061341	3.151058	1.749028
H	-2.543340	-2.559782	1.930838
H	-0.821968	-2.807270	1.925051
H	2.543340	1.067124	-0.880754
H	-0.036454	-3.151058	-0.738131
H	1.357125	2.993968	-0.530357
H	-0.160635	2.111822	-0.388894
H	-2.215658	-1.230537	-0.333874
H	-2.267710	-2.990784	-0.319106
H	-1.298380	-2.035676	-2.602071
H	0.464426	-2.083811	-2.675793
H	1.761809	0.054821	-2.753086
H	0.910393	1.600611	-2.715032
H	-1.097802	0.367097	-1.605923
H	-0.759763	0.105485	-3.288846

$Cd(L333H)^{3+}$(X)

N	0.998301	-0.403532	2.289160
C	0.998301	1.155791	2.289160
C	-0.385504	-1.084857	2.289160
Cd	2.421199	-0.905159	0.633900
C	0.730925	1.912333	0.957457
C	-1.200894	-0.876428	0.979445
N	1.913329	0.560326	-0.989947
C	1.758386	1.896616	-0.205522
C	-1.645515	-2.165080	0.242000
C	0.688749	0.172748	-1.828531
N	-2.032730	-1.824608	-1.220566

C	0.486998	-1.367268	-1.917442
C	-0.911364	-1.905321	-2.304914
H	1.422415	-0.672839	3.190683
H	1.972928	1.451336	2.701241
H	0.239244	1.471647	3.016371
H	-0.936764	-0.675521	3.144533
H	-0.213328	-2.146398	2.503183
H	0.701201	2.969076	1.264200
H	-0.282578	1.723570	0.590113
H	-0.609519	-0.271392	0.294285
H	-2.094201	-0.284132	1.213616
H	2.708016	0.688662	-1.632917
H	2.762757	2.162048	0.150911
H	1.466724	2.667193	-0.929985
H	-2.530618	-2.606603	0.711009
H	-0.875872	-2.941845	0.194528
H	0.821731	0.585099	-2.836180
H	-0.175969	0.680790	-1.395069
H	-2.480903	-0.895714	-1.240639
H	-2.762757	-2.490948	-1.525259
H	0.782901	-1.852112	-0.964579
H	1.167294	-1.777061	-2.675771
H	-1.308630	-1.396630	-3.190683
H	-0.820858	-2.969076	-2.545719

B3LYP/DZVP
$Cd(L222)^{2+}$(I)

N	0.560895	-0.760983	-1.752926
C	0.560895	0.747334	-1.752926
C	-0.808546	-1.387289	-1.752926
Cd	1.397332	-1.468717	0.279362
C	1.429057	1.385583	-0.648829
N	1.208638	0.793013	0.717800
N	-0.847931	-1.375190	0.812414
C	-1.615385	-1.131531	-0.462938
C	-0.164187	1.038629	1.291282
C	-0.882113	-0.231462	1.791201
H	1.048612	-1.093054	-2.586080
H	-0.472424	1.088997	-1.675372
H	0.932188	1.109739	-2.715154
H	-0.664288	-2.461614	-1.905057
H	-1.396206	-1.013080	-2.598751
H	1.222075	2.461614	-0.634252
H	2.491505	1.260009	-0.880428
H	1.907281	1.195912	1.343828
H	-1.237548	-2.192904	1.283501
H	-1.996624	-0.109329	-0.444826
H	-2.491505	-1.784832	-0.488233
H	-0.764623	1.545525	0.534276
H	-0.087641	1.729879	2.134767
H	-1.918525	0.035482	2.026729
H	-0.419256	-0.592324	2.715154

$Cd(L222H)^{3+}$(II)

C	1.567460	-1.030830	0.767636
C	1.567460	0.528121	0.767636
N	0.202711	-1.673932	0.767636
N	0.364893	1.180218	1.421257
C	-0.472164	-1.838098	-0.588099
Cd	-0.681641	-0.531621	2.596054
C	-0.554787	1.938724	0.486344
C	-0.358478	-0.699460	-1.606469
C	-1.683019	1.163366	-0.210028
N	-1.380570	0.441356	-1.520155
H	2.077209	-1.397989	1.665515
H	2.159431	-1.384584	-0.084138
H	1.660822	0.928754	-0.242447
H	2.462052	0.853021	1.305484
H	0.342794	-2.637978	1.089481
H	0.725195	1.886692	2.071138
H	-1.510180	-2.141838	-0.422297
H	0.020199	-2.691956	-1.069544
H	0.055416	2.494401	-0.236034
H	-1.059155	2.691956	1.099979
H	-0.525883	-1.136246	-2.596054
H	0.630325	-0.246330	-1.636969
H	-2.462052	1.887380	-0.470581
H	-2.165319	0.425799	0.441627
H	-1.108331	1.142890	-2.228012
H	-2.284824	0.084176	-1.867837
N	0.605980	-0.214778	1.882592
C	0.605980	1.307504	1.882592
C	-0.781093	-0.818141	1.882592
Cd	1.583947	-0.969188	-0.051670
C	0.907035	1.980511	0.529890
N	0.541154	0.462366	-1.491688
C	-0.903521	-2.163905	1.149252
N	-0.420919	-2.102102	-0.273994
C	0.021904	1.642327	-0.689708
C	-1.290189	-1.282810	-1.193200
C	-0.505348	-0.380441	-2.165832
H	1.072766	-0.518649	2.738608
H	1.367841	1.631300	2.595653
H	-0.357698	1.648102	2.273088
H	-1.455507	-0.084861	1.439166
H	-1.115903	-0.960029	2.914775
H	1.966127	1.832825	0.260800
H	0.828547	3.057834	0.714922
H	1.150031	0.831811	-2.224497
H	-1.954997	-2.471287	1.185011
H	-0.320397	-2.939262	1.656199
H	-0.370169	-3.057834	-0.629413
H	-0.028337	2.506284	-1.358070
H	-1.003957	1.424267	-0.385976
H	-1.966127	-0.683641	-0.581498

H	-1.922397	-1.947608	-1.788821
H	-1.222069	0.254772	-2.698355
H	0.011256	-0.988650	-2.914775

$Cd(L223)^{2+}$(III)

N	0.605980	-0.214778	1.882592
C	0.605980	1.307504	1.882592
C	-0.781093	-0.818141	1.882592
Cd	1.583947	-0.969188	-0.051670
C	0.907035	1.980511	0.529890
N	0.541154	0.462366	-1.491688
C	-0.903521	-2.163905	1.149252
N	-0.420919	-2.102102	-0.273994
C	0.021904	1.642327	-0.689708
C	-1.290189	-1.282810	-1.193200
C	-0.505348	-0.380441	-2.165832
H	1.072766	-0.518649	2.738608
H	1.367841	1.631300	2.595653
H	-0.357698	1.648102	2.273088
H	-1.455507	-0.084861	1.439166
H	-1.115903	-0.960029	2.914775
H	1.966127	1.832825	0.260800
H	0.828547	3.057834	0.714922
H	1.150031	0.831811	-2.224497
H	-1.954997	-2.471287	1.185011
H	-0.320397	-2.939262	1.656199
H	-0.370169	-3.057834	-0.629413
H	-0.028337	2.506284	-1.358070
H	-1.003957	1.424267	-0.385976
H	-1.966127	-0.683641	-0.581498
H	-1.922397	-1.947608	-1.788821
H	-1.222069	0.254772	-2.698355
H	0.011256	-0.988650	-2.914775

$Cd(L223H)^{3+}$(IV)

N	0.743189	-0.561779	1.785254
C	0.743189	0.979775	1.785254
C	-0.612216	-1.240820	1.785254
Cd	2.218231	-1.121570	0.110856
C	1.769089	1.622428	0.834022
N	1.298183	0.361825	-1.381282
C	-1.116835	-1.837734	0.461346
N	-1.916183	-0.943103	-0.482271
C	1.464009	1.714514	-0.669981
C	-0.071254	0.130087	-2.007814
C	-1.312881	0.311567	-1.119230
H	1.165830	-0.832143	2.678981
H	0.960048	1.300213	2.807467
H	-0.268997	1.321811	1.563068
H	-1.352402	-0.569858	2.236065
H	-0.530348	-2.094208	2.464937

H	2.774470	1.178721	1.003192
H	1.922574	2.654609	1.177089
H	1.919049	0.393215	-2.197448
H	-1.803164	-2.654609	0.707209
H	-0.316661	-2.289022	-0.135864
H	-2.774470	-0.642587	0.007486
H	-2.268151	-1.550678	-1.239339
H	2.290357	2.238051	-1.158309
H	0.569632	2.316664	-0.849505
H	-0.167404	0.873229	-2.807467
H	-0.059050	-0.844865	-2.505777
H	-1.170658	1.036712	-0.320145
H	-2.118388	0.699834	-1.749644

$Cd(L223H)^{3+}$(V)

N	0.903766	-0.347851	1.996827
C	0.903766	1.173510	1.996827
C	-0.462897	-1.008478	1.996827
Cd	1.987902	-1.212670	0.169315
C	0.691277	1.845039	0.625697
C	-0.653467	-2.115548	0.937690
N	-0.205875	-1.731190	-0.457827
C	-0.773577	1.995126	0.142725
C	-1.185705	-0.847463	-1.220829
N	-0.974371	1.744507	-1.351035
C	-0.602101	0.383860	-1.949419
H	1.380680	-0.627228	2.860646
H	1.882830	1.475238	2.377905
H	0.161058	1.514949	2.727239
H	-1.217971	-0.232011	1.887528
H	-0.633180	-1.465864	2.976034
H	1.311169	1.336969	-0.134656
H	1.136039	2.843200	0.694223
H	-1.710382	-2.405173	0.931406
H	-0.088639	-3.014385	1.215716
H	-0.149276	-2.606603	-0.986805
H	-1.130174	3.014385	0.314569
H	-1.472386	1.334253	0.650773
H	-1.987902	-0.562721	-0.536250
H	-1.652302	-1.484600	-1.976525
H	-1.968976	1.928607	-1.556775
H	-0.472494	2.467171	-1.891095
H	-0.976508	0.421098	-2.976034
H	0.486589	0.350002	-2.025347

$Cd(L233)^{2+}$(VI)

N	0.541073	-0.303964	2.387184
C	0.541073	1.202556	2.387184
C	-0.843252	-0.938427	2.387184
Cd	1.670441	-0.830301	0.474712
C	-1.059310	-2.090696	1.388062

N	1.145621	1.343891	-0.073011
C	0.203201	1.794923	1.010125
N	0.142935	-1.796652	-0.872481
C	-1.167471	-1.719240	-0.108055
C	0.099665	-1.106535	-2.228386
C	0.572224	1.395217	-1.481317
C	0.941010	0.176675	-2.349693
H	1.017057	-0.604204	3.239226
H	1.532858	1.529553	2.716215
H	-0.184490	1.579665	3.116217
H	-1.573020	-0.147309	2.196209
H	-1.038246	-1.306899	3.397646
H	-2.012031	-2.550831	1.672542
H	-0.316554	-2.886796	1.541768
H	1.959684	1.961003	-0.053450
H	0.201823	2.886796	1.088814
H	-0.805503	1.498785	0.713529
H	0.322458	-2.788648	-1.040177
H	-1.552667	-0.702703	-0.224834
H	-1.881004	-2.382408	-0.606846
H	0.464027	-1.820163	-2.971021
H	-0.947044	-0.901284	-2.472298
H	-0.512935	1.495865	-1.402787
H	0.936349	2.304776	-1.965328
H	0.855527	0.487423	-3.397646
H	2.012031	-0.057532	-2.225997

$Cd(L233H)^{3+}$(VII)

N	0.460910	-0.049036	1.870961
C	0.460910	1.485092	1.870961
C	-0.906207	-0.748406	1.870961
Cd	1.798528	-1.361535	0.519512
C	-0.904748	-2.156161	1.243170
C	-0.572477	2.295062	1.074937
N	0.318093	-2.000205	-1.062356
N	-0.435200	2.433752	-0.446475
C	-0.981698	-2.291304	-0.291355
C	0.245003	-1.009664	-2.210033
C	-0.785467	1.218995	-1.312863
C	0.459782	0.467133	-1.821614
H	0.857355	-0.259125	2.793645
H	1.477588	1.814650	1.638847
H	0.272451	1.795526	2.905336
H	-1.617779	-0.118383	1.339616
H	-1.250287	-0.810406	2.907505
H	-1.798528	-2.662534	1.631018
H	-0.088327	-2.780049	1.657784
H	-0.479842	3.318107	1.454208
H	-1.603156	1.989553	1.259274
H	0.600531	-2.887341	-1.491146
H	0.497059	2.798120	-0.690761
H	-1.076577	3.198877	-0.707718

H	-1.764665	-1.646158	-0.695733
H	-1.268728	-3.318107	-0.530874
H	1.036691	-1.294462	-2.907505
H	-0.705421	-1.151010	-2.736876
H	-1.455105	0.606724	-0.711856
H	-1.364748	1.592251	-2.160713
H	0.843923	0.983178	-2.708377
H	1.284171	0.541396	-1.087364

$Cd(L233H)^{3+}$(VIII)

N	1.100693	-0.780578	-2.279363
C	1.100693	0.738939	-2.279363
C	-0.241570	-1.472192	-2.279363
Cd	2.053068	-1.865352	-0.484874
C	1.019087	1.406879	-0.881419
N	-0.144704	-2.084518	0.220027
C	-0.947551	-1.488152	-0.911478
C	-0.332025	2.072542	-0.533324
C	-0.588286	-1.623455	1.604339
N	-0.591825	2.181009	0.969961
C	-0.218076	-0.193341	2.055722
C	-1.191741	0.973926	1.709447
H	1.568364	-1.060117	-3.148331
H	0.291444	1.073662	-2.938757
H	2.037924	1.031212	-2.756814
H	-0.079624	-2.492992	-2.644876
H	-0.907575	-0.983074	-2.999404
H	1.800726	2.170585	-0.822918
H	1.283188	0.668741	-0.114027
H	-0.327112	-3.094880	0.216769
H	-1.214891	-0.476779	-0.619766
H	-1.881571	-2.049508	-1.022556
H	-1.199205	1.559064	-0.950657
H	-0.351793	3.094880	-0.919924
H	-0.130325	-2.325868	2.304696
H	-1.671875	-1.779514	1.667339
H	-1.267109	2.950475	1.097274
H	0.254246	2.509404	1.457906
H	0.819229	0.046015	1.791964
H	-0.195550	-0.253597	3.148331
H	-2.053068	0.661624	1.116337
H	-1.587853	1.397955	2.634831

$Cd(L333)^{2+}$(IX)

N	-0.073296	-0.084630	2.260607
C	-0.073296	1.441267	2.260607
C	-1.464532	-0.705646	2.260607
Cd	1.151700	-0.908905	0.550849
C	1.025629	2.107635	1.412598
C	-1.570009	-2.095093	1.602940
N	1.521254	0.862039	-0.779531

N	-0.274640	-2.180797	-0.625801
C	0.853953	2.055111	-0.122096
C	-1.627485	-2.128036	0.060542
C	-0.310568	-1.713109	-2.067987
C	1.020783	0.578495	-2.181933
C	-0.317150	-0.183727	-2.271229
H	0.367211	-0.372428	3.136960
H	0.012277	1.784437	3.295125
H	-1.051290	1.767684	1.899668
H	-2.128207	-0.011861	1.739228
H	-1.814277	-0.762417	3.295423
H	2.024759	1.752835	1.706292
H	1.018702	3.164804	1.700582
H	-2.513835	-2.522707	1.959450
H	-0.799670	-2.780551	1.985552
H	2.513835	1.094217	-0.865234
H	0.003983	-3.164804	-0.645897
H	1.268471	2.960878	-0.575681
H	-0.206781	2.028703	-0.385687
H	-2.150287	-1.243179	-0.310856
H	-2.203101	-2.997476	-0.271752
H	-1.203417	-2.138826	-2.538592
H	0.556015	-2.156184	-2.568673
H	1.808540	0.015146	-2.691783
H	0.921016	1.535424	-2.705773
H	-1.081995	0.292291	-1.645356
H	-0.673042	-0.026595	-3.295423

$Cd(L333H)^{3+}$(X)

N	1.055303	-0.411655	2.263252
C	1.055303	1.128196	2.263252
C	-0.306229	-1.095929	2.263252
Cd	2.501251	-0.949770	0.615172
C	0.783695	1.884316	0.942315
C	-1.116388	-0.857024	0.965127
N	1.915304	0.527354	-1.004008
C	1.787057	1.850889	-0.229452
C	-1.668130	-2.105864	0.251799
C	0.697537	0.169135	-1.838166
N	-2.037000	-1.751666	-1.194159
C	0.460298	-1.357510	-1.941980
C	-0.951184	-1.865215	-2.287489
H	1.467805	-0.669798	3.167481
H	2.033128	1.418247	2.663944
H	0.308557	1.446180	2.999632
H	-0.853972	-0.719031	3.133139
H	-0.118467	-2.158235	2.444456
H	0.782100	2.938577	1.250559
H	-0.237558	1.721544	0.592443
H	-0.477931	-0.329721	0.263848
H	-1.948639	-0.177814	1.178766
H	2.696454	0.660760	-1.654865

H	2.797542	2.099851	0.114021
H	1.502854	2.624999	-0.950293
H	-2.580843	-2.474084	0.726400
H	-0.962629	-2.938577	0.200534
H	0.840819	0.589666	-2.838801
H	-0.154686	0.693041	-1.405229
H	-2.465707	-0.816801	-1.213042
H	-2.797542	-2.380276	-1.494659
H	0.780632	-1.864068	-1.013559
H	1.105238	-1.772433	-2.724845
H	-1.361656	-1.362508	-3.167481
H	-0.888128	-2.931334	-2.515148

B3LYP/LanL2DZ
$Ni(L222)^{2+}$(I)

N	0.646608	-0.680530	-1.907049
C	0.646608	0.843969	-1.907049
C	-0.695625	-1.397207	-1.907049
Ni	1.425808	-1.178119	-0.143339
C	0.446288	1.436883	-0.491483
N	1.269423	0.686381	0.549870
N	-0.397560	-1.538443	0.633480
C	-1.385173	-1.338229	-0.525627
C	0.585523	0.479444	1.891497
C	-0.582094	-0.548836	1.790624
H	1.174519	-0.997634	-2.729376
H	-0.133286	1.222345	-2.578874
H	1.614103	1.156194	-2.316019
H	-0.496910	-2.434640	-2.200682
H	-1.359709	-0.962579	-2.664267
H	-0.601429	1.398586	-0.187168
H	0.737114	2.492893	-0.502086
H	2.161250	1.172973	0.702951
H	-0.505709	-2.492893	0.996292
H	-2.161250	-2.109297	-0.480071
H	-1.881727	-0.376879	-0.382302
H	0.206790	1.432636	2.278894
H	1.355309	0.126224	2.587451
H	-0.636408	-1.108099	2.729376
H	-1.544035	-0.045090	1.664897

$Ni(L222H)^{2+}$(II)

N	1.067440	-0.641946	-1.731730
C	1.067440	0.893988	-1.731730
C	-0.302749	-1.346295	-1.731730
Ni	2.365865	-0.962445	-0.245399
C	0.956128	1.485529	-0.296190
N	1.521888	0.531999	0.779011
C	-1.401535	-0.804872	-0.799206
N	-1.430969	-1.344839	0.653965

C	0.518978	0.013065	1.819881
C	-0.154602	-1.344896	1.516876
H	1.517429	-0.950823	-2.610363
H	0.257677	1.272018	-2.368299
H	2.005405	1.206409	-2.208620
H	-0.133203	-2.423673	-1.606159
H	-0.697059	-1.222517	-2.751299
H	-0.072591	1.730404	-0.024060
H	1.519395	2.423673	-0.256228
H	2.242401	1.049340	1.307520
H	-2.365865	-1.106828	-1.226437
H	-1.418177	0.284149	-0.744321
H	-2.168522	-0.817171	1.155919
H	-1.772604	-2.322883	0.627480
H	-0.215837	0.802337	2.025743
H	1.081027	-0.129484	2.751299
H	0.528397	-2.085182	1.068104
H	-0.456454	-1.782231	2.477804

Ni(L223)$^{2+}$(III)

N	0.412984	-0.168648	1.826305
C	0.412984	1.369815	1.826305
C	-0.983183	-0.792502	1.826305
Ni	1.303027	-0.925949	0.203587
C	0.911996	2.007653	0.508460
N	0.817477	0.250361	-1.325136
C	-0.973355	-2.189983	1.177149
N	-0.257705	-2.135448	-0.165471
C	0.205014	1.544115	-0.785680
C	-1.039953	-1.451999	-1.283701
C	-0.104558	-0.611516	-2.177926
H	0.905573	-0.483931	2.673207
H	1.052334	1.706373	2.648662
H	-0.606022	1.703797	2.049518
H	-1.644978	-0.113408	1.282582
H	-1.362824	-0.861392	2.851831
H	2.002750	1.883350	0.404319
H	0.762487	3.089888	0.613168
H	1.639618	0.506066	-1.888406
H	-2.002750	-2.547368	1.052537
H	-0.444427	-2.918457	1.803217
H	-0.010541	-3.089888	-0.454003
H	0.293869	2.311865	-1.562684
H	-0.863375	1.373173	-0.619881
H	-1.810431	-0.825509	-0.826598
H	-1.553763	-2.203079	-1.893007
H	0.527783	-1.257106	-2.798465
H	-0.698903	0.016852	-2.851831

Ni(L223H)$^{3+}$(IV)

N 0	0.683046	-0.370986	1.812917
C 0	0.683046	1.179588	1.812917
C 0	-0.676526	-1.086125	1.812917
Ni 0	1.993044	-0.700139	0.357209
C 0	1.750817	1.740951	0.834354
N	1.329976	0.289438	-1.234258
C	-1.011651	-1.937806	0.566310
N	-1.830754	-1.238328	-0.536955
C	1.395790	1.733538	-0.676993
C	0.039231	-0.090163	-1.972000
C	-1.285547	0.048577	-1.192328
H	1.157359	-0.665232	2.682892
H	0.898159	1.518182	2.832133
H	-0.316428	1.538873	1.554116
H	-1.458862	-0.349493	2.032513
H	-0.667601	-1.777661	2.662951
H	2.763293	1.289413	1.026273
H	1.948055	2.787231	1.115954
H	2.073155	0.197050	-1.948743
H	-1.628051	-2.787231	0.885547
H	-0.124066	-2.372482	0.088527
H	-2.013179	-1.937842	-1.278931
H	-2.763293	-1.006812	-0.149383
H	2.163713	2.277316	-1.237886
H	0.442629	2.238244	-0.855825
H	0.173444	-1.095091	-2.393049
H	-0.026163	0.590526	-2.832133
H	-1.250086	0.814574	-0.414826
H	-2.064651	0.354421	-1.900326

$Ni(L223H)^{3+}$(V)

N	1.929708	-0.730578	1.227776
C	1.929708	0.820157	1.227776
C	0.576027	-1.495468	1.227776
C	1.288678	1.488303	-0.015411
C	0.071375	-2.089338	-0.109857
N	-0.781857	-1.231924	-1.069779
C	-0.228482	1.868057	0.111040
Ni	0.061109	0.247992	-2.150373
N	-1.013019	1.575978	-1.164679
C	-2.045654	-0.607475	-0.431136
C	-2.324755	0.811975	-0.978631
H	2.539537	-1.078173	0.469745
H	2.414494	-0.999548	2.103951
H	2.984535	1.105582	1.305038
H	1.432166	1.138525	2.150373
H	-0.148881	-0.857942	1.738235
H	0.739837	-2.359617	1.882224
H	1.514806	0.826509	-0.903747
H	1.870596	2.389694	-0.244782
H	-0.568736	-2.935976	0.177887

H	0.893079	-2.521114	-0.696915
H	-1.103401	-1.910768	-1.780990
H	-0.316299	2.935976	0.337395
H	-0.706133	1.329929	0.932476
H	-1.197362	2.449453	-1.680830
H	-1.912711	-0.594093	0.651356
H	-2.907833	-1.251506	-0.637229
H	-2.830088	0.787527	-1.952664
H	-2.984535	1.355494	-0.290073

Ni(L233)$^{2+}$(VI)

N	0.236682	-0.174032	2.284642
C	0.236682	1.352557	2.284642
C	-1.160556	-0.799643	2.284642
Ni	1.264785	-0.624481	0.628667
C	-1.235429	-2.155241	1.550874
N	1.047408	1.224371	-0.085994
C	0.039123	1.877391	0.848870
N	0.240906	-1.858376	-0.533733
C	-1.175349	-2.058748	0.011812
C	0.279215	-1.387063	-1.999025
C	0.654876	1.168362	-1.563545
C	1.146937	-0.130611	-2.242723
H	0.726413	-0.502840	3.127103
H	1.192994	1.691140	2.701689
H	-0.559154	1.733006	2.935462
H	-1.845297	-0.085425	1.815021
H	-1.476991	-0.918238	3.327386
H	-2.204762	-2.601626	1.807760
H	-0.484744	-2.860994	1.939033
H	1.941639	1.729874	-0.014208
H	0.140974	2.968180	0.829092
H	-0.960836	1.633177	0.478106
H	0.711569	-2.773990	-0.488057
H	-1.779744	-1.215462	-0.338912
H	-1.586765	-2.968180	-0.442716
H	-0.751886	-1.195235	-2.312537
H	0.659176	-2.211409	-2.611668
H	1.078238	2.041869	-2.071230
H	-0.435209	1.249412	-1.627621
H	1.148203	0.039682	-3.327386
H	2.204762	-0.323100	-1.990799

Ni(L233H)$^{3+}$(VII)

N	0.379843	-0.148830	1.717288
C	0.379843	1.391060	1.717288

C	-1.020277	-0.811718	1.717288
Ni	1.450034	-1.315592	0.491882
C	-0.944740	-2.285792	1.244803
C	-0.218539	2.168771	0.518951
N	0.255389	-1.848188	-0.974639
N	0.773747	2.630717	-0.586999
C	-0.941920	-2.532150	-0.286797
C	-0.073310	-0.573779	-1.736676
C	0.809074	1.876160	-1.942408
C	1.160308	0.372392	-1.836141
H	0.797166	-0.382866	2.636794
H	1.404832	1.718353	1.936459
H	-0.220089	1.680469	2.591754
H	-1.689149	-0.223916	1.083412
H	-1.411078	-0.764271	2.740742
H	-1.818048	-2.817419	1.648736
H	-0.095381	-2.814762	1.736186
H	-0.629312	3.095352	0.934551
H	-1.047208	1.660115	0.023720
H	0.713436	-2.521858	-1.608945
H	0.522005	3.607209	-0.823522
H	1.731375	2.685013	-0.204045
H	-1.864975	-2.167840	-0.749773
H	-0.873485	-3.607209	-0.481154
H	-0.910247	-0.100004	-1.219476
H	-0.426491	-0.839016	-2.740742
H	1.558110	2.402773	-2.543323
H	-0.165782	2.030418	-2.417236
H	1.766576	0.105375	-2.710027
H	1.864975	0.240974	-0.973626

Ni(L233H)$^{3+}$(VIII)

N	1.378531	-0.502261	2.354150
C	1.378531	1.029643	2.354150
C	0.015451	-1.207263	2.354150
Ni	2.317903	-0.912229	0.645247
C	-0.480025	-1.588994	0.919194
N	1.980018	0.915951	-0.103235
C	1.083103	1.580677	0.946597
C	-1.731283	-0.799560	0.445841
C	1.494665	1.045019	-1.563887
N	-1.896665	-0.732701	-1.085034
C	0.422411	0.054015	-2.098418
C	-1.088550	0.362816	-1.840359
H	1.897658	-0.820012	3.187004
H	2.363458	1.355538	2.711621
H	0.637219	1.402326	3.071326
H	-0.705697	-0.566645	2.875967
H	0.130555	-2.114078	2.955210
H	-0.693565	-2.664333	0.888764
H	0.339032	-1.444900	0.174071
H	2.894964	1.398264	-0.079269

H	1.250880	2.664333	0.933243
H	0.046380	1.405662	0.657596
H	-1.740740	0.235797	0.796218
H	-2.629795	-1.285884	0.843598
H	2.392154	0.925239	-2.181009
H	1.157288	2.082648	-1.695300
H	-1.723622	-1.656669	-1.514580
H	-2.894964	-0.527534	-1.268013
H	0.676332	-0.989116	-1.855916
H	0.557775	0.097195	-3.187004
H	-1.253732	1.293749	-1.289711
H	-1.601223	0.467266	-2.802010

$Ni(L333)^{2+}$(IX)

N	-0.225854	-0.117300	2.224732
C	-0.225854	1.416622	2.224732
C	-1.642835	-0.705551	2.224732
Ni	0.944906	-0.897526	0.805630
C	1.049367	2.049025	1.633579
C	-1.740385	-2.121890	1.624905
N	1.740578	0.540338	-0.313643
N	-0.078117	-2.178855	-0.318548
C	1.186754	1.901251	0.103491
C	-1.548233	-2.184046	0.094919
C	0.126153	-1.911698	-1.812413
C	1.573512	0.254419	-1.808512
C	0.230676	-0.414273	-2.167752
H	0.223257	-0.417710	3.103957
H	-0.375433	1.759452	3.255473
H	-1.095139	1.737783	1.642460
H	-2.274997	-0.021594	1.649926
H	-2.013049	-0.706487	3.256906
H	1.955691	1.694877	2.150819
H	0.999401	3.122388	1.857198
H	-2.752253	-2.486159	1.844151
H	-1.068697	-2.827542	2.139939
H	2.752253	0.560449	-0.115943
H	0.288002	-3.122388	-0.121928
H	1.858964	2.671416	-0.294203
H	0.215369	2.028240	-0.385948
H	-2.031653	-1.329461	-0.390204
H	-2.006245	-3.094777	-0.309966
H	-0.713304	-2.366713	-2.351956
H	1.036583	-2.439262	-2.120599
H	2.409899	-0.383397	-2.118017
H	1.672876	1.205955	-2.344764
H	-0.615251	0.150505	-1.750609
H	0.118685	-0.337540	-3.256906

$Ni(L333H)^{3+}$(X)

N	1.067440	-0.641946	-1.731730
C	1.067440	0.893988	-1.731730
C	-0.302749	-1.346295	-1.731730
Ni	2.365865	-0.962445	-0.245399
C	0.956128	1.485529	-0.296190
N	1.521888	0.531999	0.779011
C	-1.401535	-0.804872	-0.799206
N	-1.430969	-1.344839	0.653965
C	0.518978	0.013065	1.819881
C	-0.154602	-1.344896	1.516876
H	1.517429	-0.950823	-2.610363
H	0.257677	1.272018	-2.368299
H	2.005405	1.206409	-2.208620
H	-0.133203	-2.423673	-1.606159
H	-0.697059	-1.222517	-2.751299
H	-0.072591	1.730404	-0.024060
H	1.519395	2.423673	-0.256228
H	2.242401	1.049340	1.307520
H	-2.365865	-1.106828	-1.226437
H	-1.418177	0.284149	-0.744321
H	-2.168522	-0.817171	1.155919
H	-1.772604	-2.322883	0.627480
H	-0.215837	0.802337	2.025743
H	1.081027	-0.129484	2.751299
H	0.528397	-2.085182	1.068104
H	-0.456454	-1.782231	2.477804

B3LYP/DZVP2

$Ni(L222)^{2+}$(I)

N	-0.641587	-1.886575	-0.678874
C	-0.647190	-1.889915	0.830646
C	0.685151	-1.888046	-1.392530
Ni	-1.427030	-0.141829	-1.180874
C	-0.442790	-0.481284	1.420367
N	-1.259043	0.546523	0.672406
N	0.389356	0.632419	-1.529127
C	1.372791	-0.512820	-1.340303
C	-0.590021	1.878037	0.468501
C	0.578840	1.777368	-0.548340
H	-1.154726	-2.714442	-0.988922
H	0.118940	-2.569948	1.215164
H	-1.621156	-2.284310	1.131485
H	0.474432	-2.174447	-2.426697
H	1.349487	-2.647599	-0.968715
H	0.602927	-0.179800	1.375958
H	-0.727916	-0.487237	2.475095
H	-2.141230	0.701548	1.165642
H	0.505971	0.999488	-2.475095
H	2.141230	-0.467612	-2.115101
H	1.876182	-0.369433	-0.385329
H	-0.227155	2.279611	1.419470
H	-1.362033	2.558812	0.099019

H	0.640687	2.714442	-1.104026
H	1.535623	1.643791	-0.042573

$Ni(L222H)^{3+}$(II)

N	-1.017700	-1.721887	-0.665586
C	-1.039120	-1.776511	0.854731
C	0.355385	-1.678903	-1.338464
Ni	-2.400647	-0.265526	-0.942608
C	-0.964456	-0.364932	1.485184
N	-1.526367	0.715762	0.556549
C	1.434926	-0.765709	-0.745139
N	1.468385	0.696191	-1.203467
C	-0.545670	1.788490	0.102674
C	0.213143	1.564200	-1.216630
H	-1.431612	-2.600189	-1.004794
H	-0.228027	-2.414096	1.221855
H	-1.975147	-2.270299	1.131805
H	0.205345	-1.515502	-2.410099
H	0.754395	-2.696316	-1.240637
H	0.052266	-0.078750	1.753427
H	-1.545491	-0.356973	2.410099
H	-2.248357	1.219915	1.086091
H	2.400647	-1.174030	-1.058840
H	1.444489	-0.766880	0.343492
H	2.191373	1.168380	-0.639835
H	1.845655	0.723235	-2.162593
H	0.132586	2.005304	0.935591
H	-1.135904	2.696316	-0.055571
H	-0.423517	1.183299	-2.022749
H	0.556409	2.547875	-1.553875

$Ni(L223)^{2+}$(III)

N	-0.440360	-1.418699	0.498071
C	-1.811611	-1.038781	-0.046529
C	0.559172	-1.816843	-0.567037
Ni	0.434735	0.057854	1.500924
C	-2.159929	0.454768	0.098459
N	-0.012928	1.715741	0.521452
C	1.998055	-1.554762	-0.103847
N	2.114374	-0.157203	0.444573
C	-1.133914	1.455006	-0.463272
C	2.088573	0.942970	-0.592023
C	1.299947	2.156028	-0.075187
H	-0.570147	-2.224544	1.115484
H	-2.559123	-1.630099	0.485839
H	-1.848191	-1.339054	-1.096276
H	0.328479	-1.239273	-1.462924
H	0.436507	-2.872363	-0.823471
H	-2.378541	0.699788	1.147665
H	-3.107922	0.603984	-0.428043
H	-0.332523	2.453864	1.154072
H	2.692031	-1.707765	-0.936151
H	2.286075	-2.241508	0.697470
H	2.981292	-0.088897	0.981792

H	-1.618948	2.409721	-0.683363
H	-0.692382	1.095371	-1.395017
H	1.637197	0.543629	-1.500924
H	3.107922	1.244582	-0.844004
H	1.857055	2.669389	0.713487
H	1.134820	2.872363	-0.885376

$Ni(L223H)^{3+}$(IV)

N	0.667146	-0.334898	1.811132
C	0.667146	1.196503	1.811132
C	-0.673339	-1.055066	1.811132
Ni	2.006103	-0.627893	0.392466
C	1.732778	1.734545	0.826367
N	1.324577	0.301615	-1.212838
C	-0.992043	-1.926669	0.582198
N	-1.782914	-1.263382	-0.541737
C	1.372592	1.733839	-0.676075
C	0.069685	-0.101070	-1.965489
C	-1.270242	0.005725	-1.219512
H	1.127542	-0.619312	2.683927
H	0.890226	1.538608	2.824648
H	-0.328040	1.560998	1.553029
H	-1.464010	-0.326866	2.014663
H	-0.661314	-1.736154	2.665661
H	2.726523	1.230290	1.000488
H	1.996955	2.760787	1.115586
H	2.071458	0.219168	-1.915407
H	-1.619481	-2.760787	0.910607
H	-0.103032	-2.380551	0.132712
H	-1.946150	-1.981164	-1.263359
H	-2.726523	-1.047771	-0.186994
H	2.134386	2.281245	-1.236484
H	0.417372	2.231314	-0.849570
H	0.234131	-1.100326	-2.381245
H	0.001753	0.576176	-2.824648
H	-1.285918	0.797918	-0.470786
H	-2.041673	0.256265	-1.953150

$Ni(L223H)^{3+}$(V)

N	1.912845	-0.768077	1.194539
C	1.912845	0.764625	1.194539
C	0.592458	-1.558674	1.194539
C	1.284890	1.450459	-0.039682
C	0.065440	-2.107851	-0.144056
N	-0.742987	-1.214390	-1.077673
C	-0.220267	1.864493	0.075530
Ni	0.130567	0.261668	-2.114102
N	-0.991020	1.565576	-1.187361
C	-1.995136	-0.601100	-0.446911
C	-2.282397	0.798569	-1.017967
H	2.537398	-1.117971	0.455996
H	2.397736	-1.030420	2.066017
H	2.966271	1.043825	1.276025
H	1.413792	1.080981	2.114102

H	-0.130818	-0.969382	1.758749
H	0.801583	-2.446261	1.798265
H	1.521227	0.795045	-0.930221
H	1.886474	2.336410	-0.265662
H	-0.597497	-2.935589	0.135634
H	0.871384	-2.556718	-0.734379
H	-1.068947	-1.866429	-1.803250
H	-0.283415	2.935589	0.281384
H	-0.707945	1.351126	0.903181
H	-1.178986	2.431338	-1.705565
H	-1.849731	-0.561102	0.630980
H	-2.852000	-1.254865	-0.630065
H	-2.756405	0.749130	-2.003686
H	-2.966271	1.343347	-0.357655

$Ni(L233)^{2+}$(VI)

N	0.198898	-0.152460	2.266496
C	0.198898	1.357888	2.266496
C	-1.178610	-0.784152	2.266496
Ni	1.250832	-0.608374	0.645393
C	-1.237853	-2.136357	1.538436
N	1.064290	1.232008	-0.062983
C	0.041578	1.882357	0.832711
N	0.207531	-1.786281	-0.538090
C	-1.182498	-2.045292	0.005750
C	0.223496	-1.292351	-1.979814
C	0.741954	1.225383	-1.544101
C	1.154494	-0.091622	-2.225543
H	0.676118	-0.466423	3.114821
H	1.147902	1.688363	2.699020
H	-0.604181	1.742825	2.901367
H	-1.868478	-0.078657	1.797592
H	-1.493662	-0.903738	3.306481
H	-2.198053	-2.594081	1.796909
H	-0.477747	-2.828214	1.924937
H	1.952381	1.727713	0.056779
H	0.143188	2.970889	0.815139
H	-0.945335	1.636737	0.435064
H	0.691955	-2.689222	-0.528169
H	-1.823097	-1.232536	-0.344487
H	-1.555790	-2.970889	-0.442182
H	-0.801209	-1.030536	-2.250580
H	0.528211	-2.122729	-2.620862
H	1.256829	2.065874	-2.015449
H	-0.331175	1.395480	-1.655099
H	1.157730	0.083963	-3.306481
H	2.198053	-0.343149	-1.981348

$Ni(L233H)^{3+}$(VII)

N	0.414289	-0.057417	1.655243
C	0.595231	1.453451	1.621916
C	-1.041975	-0.533838	1.685082
C	-1.163281	-2.026588	1.325927

N	1.169472	2.499489	-0.725051
C	0.137785	2.267022	0.394861
N	0.123916	-1.888041	-0.871409
C	-1.137284	-2.386563	-0.174066
C	-0.041006	-0.643295	-1.698479
C	1.145323	1.661217	-2.007792
C	1.296019	0.138736	-1.809188
Ni	1.405732	-1.316734	0.479786
H	0.789467	-0.308556	2.580612
H	1.641528	1.665256	1.865744
H	0.008738	1.841710	2.462808
H	-1.626312	0.089010	1.006265
H	-1.421226	-0.360715	2.696810
H	-2.119192	-2.390513	1.720199
H	-0.415485	-2.620147	1.883386
H	1.039269	3.472392	-1.039079
H	2.119192	2.494602	-0.330842
H	-0.083973	3.267351	0.774834
H	-0.778231	1.906479	-0.072912
H	0.499128	-2.642282	-1.459082
H	-2.002403	-1.972734	-0.698433
H	-1.167839	-3.472392	-0.283825
H	-0.818296	-0.045254	-1.224369
H	-0.401944	-0.910137	-2.696810
H	1.968859	2.047729	-2.612791
H	0.212175	1.900441	-2.524076
H	1.892983	-0.253939	-2.638013
H	1.973832	-0.018767	-0.924215

Ni(L233H)$^{3+}$(VIII)

N	1.379824	-0.479919	2.356449
C	1.379824	1.034546	2.356449
C	0.037344	-1.184973	2.356449
Ni	2.269356	-0.891478	0.644243
C	-0.426858	-1.586418	0.922133
N	1.933824	0.924617	-0.089166
C	1.061274	1.583360	0.960238
C	-1.685909	-0.838244	0.426282
C	1.456300	1.077395	-1.531460
N	-1.843335	-0.798571	-1.087353
C	0.431993	0.067114	-2.103760
C	-1.091120	0.291549	-1.870650
H	1.898551	-0.791522	3.185076
H	2.373642	1.352706	2.686509
H	0.658923	1.410160	3.089492
H	-0.696985	-0.546531	2.856106
H	0.152152	-2.082273	2.966276
H	-0.601416	-2.665587	0.883728
H	0.394483	-1.419487	0.182820
H	2.843490	1.403538	-0.062177
H	1.222207	2.665587	0.943858
H	0.022021	1.403186	0.689560
H	-1.726622	0.198885	0.761190
H	-2.571587	-1.342286	0.824023

H	2.358576	1.002379	-2.142813
H	1.087140	2.103535	-1.638987
H	-1.655584	-1.722364	-1.499942
H	-2.843490	-0.637109	-1.274470
H	0.726974	-0.971119	-1.903367
H	0.575989	0.157545	-3.185076
H	-1.319088	1.234239	-1.369099
H	-1.597442	0.316290	-2.837584

$Ni(L333)^{2+}$(IX)

N	-0.244347	-0.106273	2.209791
C	-0.244347	1.411060	2.209791
C	-1.644184	-0.691598	2.209791
Ni	0.960149	-0.906917	0.851843
C	1.029593	2.039321	1.629282
C	-1.732378	-2.107873	1.625575
N	1.742883	0.515015	-0.273195
N	-0.050188	-2.175127	-0.275807
C	1.194249	1.869561	0.110623
C	-1.511808	-2.189347	0.106666
C	0.184156	-1.946525	-1.754957
C	1.622562	0.212896	-1.753136
C	0.301273	-0.465426	-2.145006
H	0.187345	-0.393684	3.094925
H	-0.398897	1.754718	3.236607
H	-1.108553	1.731792	1.624698
H	-2.273511	-0.017187	1.625803
H	-2.020760	-0.683246	3.236612
H	1.926748	1.696477	2.163126
H	0.970781	3.112743	1.835033
H	-2.745294	-2.468284	1.830712
H	-1.069543	-2.804610	2.157203
H	2.745294	0.545883	-0.061566
H	0.306114	-3.112743	-0.064737
H	1.876491	2.629481	-0.282198
H	0.235484	1.995884	-0.398018
H	-1.996034	-1.350555	-0.399090
H	-1.951212	-3.109838	-0.289401
H	-0.640128	-2.412833	-2.302699
H	1.098291	-2.481550	-2.026240
H	2.468467	-0.424340	-2.025118
H	1.735659	1.153907	-2.299580
H	-0.559580	0.107119	-1.779995
H	0.234801	-0.420055	-3.236612

$Ni(L333H)^{3+}$(X)

N	1.177011	0.122006	1.981385
C	1.177011	1.651325	1.981385
C	-0.181183	-0.547898	1.981385
Ni	2.295095	-0.190068	0.402483
C	1.884660	2.211975	0.721740
C	-0.182490	-1.879279	1.192090
N	1.488593	0.623998	-1.195804

C	1.189552	2.017792	-0.651522
C	-1.591540	-2.317657	0.696429
C	0.429845	-0.101653	-2.018879
N	-1.675738	-2.494882	-0.820834
C	-1.005656	-0.038495	-1.444781
C	-1.914258	-1.253041	-1.698421
H	1.686735	-0.196533	2.813649
H	1.709624	1.992752	2.871590
H	0.149021	2.011376	2.047204
H	-0.887067	0.166017	1.557994
H	-0.481483	-0.715215	3.019927
H	2.948435	1.855155	0.677063
H	2.040957	3.286043	0.884931
H	0.242840	-2.678819	1.803965
H	0.479290	-1.788415	0.313414
H	2.286322	0.728426	-1.836779
H	1.562553	2.756582	-1.365452
H	0.112189	2.150736	-0.564990
H	-2.376339	-1.609718	0.971062
H	-1.858384	-3.286043	1.122861
H	0.797328	-1.126220	-2.136762
H	0.444944	0.341689	-3.019927
H	-2.473069	-3.119713	-1.006676
H	-0.860927	-3.024678	-1.150641
H	-1.003404	0.189487	-0.379279
H	-1.532658	0.797743	-1.913443
H	-2.948435	-0.962965	-1.502617
H	-1.859887	-1.605488	-2.732007