Electronic supplementary information (ESI)

For

Electrospray ionization photoelectron spectroscopy of cryogenic $[EDTA•M(II)]^{2-}$ complexes (M = Ca, V−Zn): electronic structures and intrinsic redox properties

Qinqin Yuan,[#1,2,3,§] Xiang-Tao Kong,[#2] Gao-Lei Hou,[1] Ling Jiang,*[2] and Xue-Bin Wang*[1]

[1]Physical Sciences Division, Pacific Northwest National Laboratory, 902 Battelle Boulevard, P. O. Box 999, MS K8-88, Richland, Washington 99352, USA

[2]State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 457 Zhongshan Road, Dalian 116023, China

[3]University of Chinese Academy of Sciences, 19A Yuquan Road, Beijing 100049, China

Contents

Table S1 Comparison of the experimental VDE values to the calculated ones (eV) obtained using different functionals for [EDTA•*M* (II)]$^{2-}$ (*M* = Ca, Mn, Co, Ni, Cu, and Zn).

Methods	Ca(II)	Mn(II)	Co(II)	Ni(II)	Cu(II)	Zn(II)	Avg. deviation
Expt. VDE (eV)	**2.70**	**1.15**	**1.7**	**1.73**	**1.78**	**2.2**	
PBE0/6-311+G(d,p)	2.08	1.15	1.21	1.59	1.39	1.82	
	-0.62	0	-0.49	-0.14	-0.39	-0.38	
	-22.96%	0.00%	-28.82%	-8.09%	-21.91%	-17.27%	16.50%
B3LYP/6-311+G(d,p)	2.00	1.06	1.23	1.53	1.38	1.77	
	-0.70	-0.09	-0.47	-0.2	-0.4	-0.43	
	-25.93%	-7.83%	-27.65%	-11.56%	-22.47%	-19.55%	19.17%
MN12SX/6-311+G(d,p)	**2.33**	**1.16**	**1.64**	**1.63**	**1.66**	**2.08**	
	-0.37	0.01	-0.06	-0.1	-0.12	-0.12	
	-13.70%	0.87%	-3.53%	-5.78%	-6.74%	-5.45%	6.01%
BP86/6-311+G(d,p)	1.35	0.21	0.42	0.5	0.57	1.14	
	-1.35	-0.94	-1.28	-1.23	-1.21	-1.06	
	-50.00%	-81.74%	-75.29%	-71.10%	-67.98%	-48.18%	65.72%
MN15/6-311+G(d,p)	2.62	1.4	1.31	1.71	1.82	2.29	
	-0.08	0.25	-0.39	-0.02	0.04	0.09	
	-2.96%	21.74%	-22.94%	-1.16%	2.25%	4.09%	9.19%

Table S2 Comparison of relative energies (RE) for the hexadentate [EDTA•*M*(II)]$^{2-}$ (*M* = Mn, Co, and Ni) complexes of different spin states at the MN12SX/6-311+G(d,p) level.

Cluster	Isomer	RE (eV)
[EDTAMn(II)]$^{2-}$	Iso A	
	^{6}A	0.00
	^{4}A	+1.11
	^{2}A	+1.27
[EDTACo(II)]$^{2-}$	Iso A	
	^{4}A	+0.00
	^{2}A	+0.39
[EDTANi(II)]$^{2-}$	Iso A	
	^{3}A	+0.00
	^{1}A	+0.87

Table S3 Comparison of relative energies (RE) of different isomers for the [EDTA•*M*(II)]$^{2-}$ (*M* = Ca, V − Zn) complexes at the MN12SX/6-311+G(d,p) level.

Cluster		Isomer	State	RE (eV)
[EDTACa(II)]$^{2-}$	hexadentate	Iso A	^{1}A	0
	pentadentate	Iso B	^{1}A	0.75
	tetradentate	Iso C	^{1}A	1.88
[EDTAV(II)]$^{2-}$	hexadentate	Iso A	^{4}A	0
	pentadentate	Iso B	^{4}A	0.73
	tetradentate	Iso C	^{4}A	1.59
[EDTACr(II)]$^{2-}$	hexadentate	Iso A	^{5}A	0
	pentadentate	Iso B	^{5}A	0.44
	tetradentate	Iso C	^{5}A	0.83
[EDTAMn(II)]$^{2-}$	hexadentate	Iso A	^{6}A	0
	pentadentate	Iso B	^{6}A	0.42
	tetradentate	Iso C	^{6}A	1.35
[EDTAFe(II)]$^{2-}$	hexadentate	Iso A	^{5}A	0
	pentadentate	Iso B	^{5}A	0.25
	tetradentate	Iso C	^{5}A	0.93
[EDTACo(II)]$^{2-}$	hexadentate	Iso A	^{4}A	0
	pentadentate	Iso B	^{4}A	0.15
	tetradentate	Iso C	^{4}A	0.91
[EDTANi(II)]$^{2-}$	hexadentate	Iso A	^{3}A	0
	pentadentate	IsoB	^{3}A	0.34
	tetradentate	Iso C	^{3}A	0.79
[EDTACu(II)]$^{2-}$	hexadentate	Iso A	^{2}A	0
	pentadentate	Iso B	^{2}A	0.06
	tetradentate	Iso C	^{2}A	0.21
[EDTAZn(II)]$^{2-}$	hexadentate	Iso A	^{1}A	0
	pentadentate	Iso B	^{1}A	0.23
	tetradentate	Iso C	^{1}A	0.82

Table S4 Energy barriers for Iso A transforming into Iso B of the [EDTA•*M*(II)]$^{2-}$ (*M* = Ca, Mn, Co, Ni, Cu, and Zn) complexes at the MN12SX/6-311+G(d,p) level.

[EDTA•*M*(II)]$^{2-}$	Energy barrier between Iso A and Iso B (eV)
Ca	1.34
Mn	1.09
Co	0.86
Ni	1.05
Cu	0.29
Zn	0.91

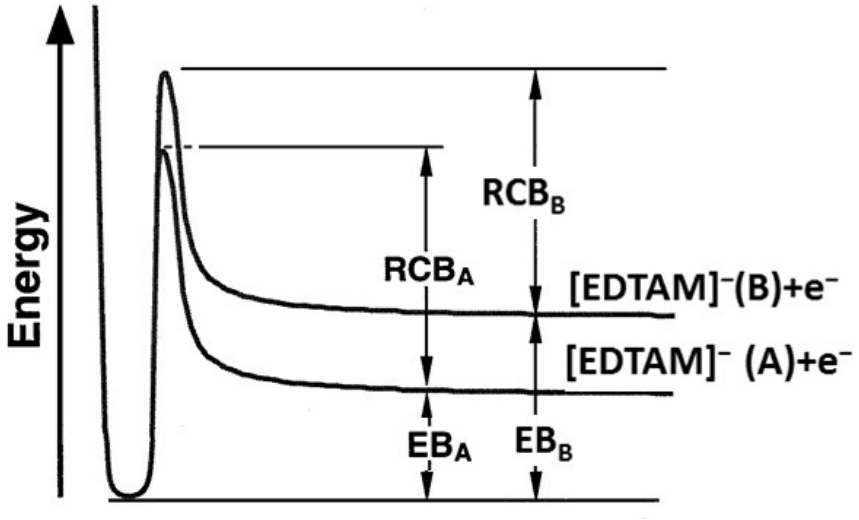

Fig. S1 Schematic potential energy curves explaining the RCB effects in the observed photoelectron spectra.

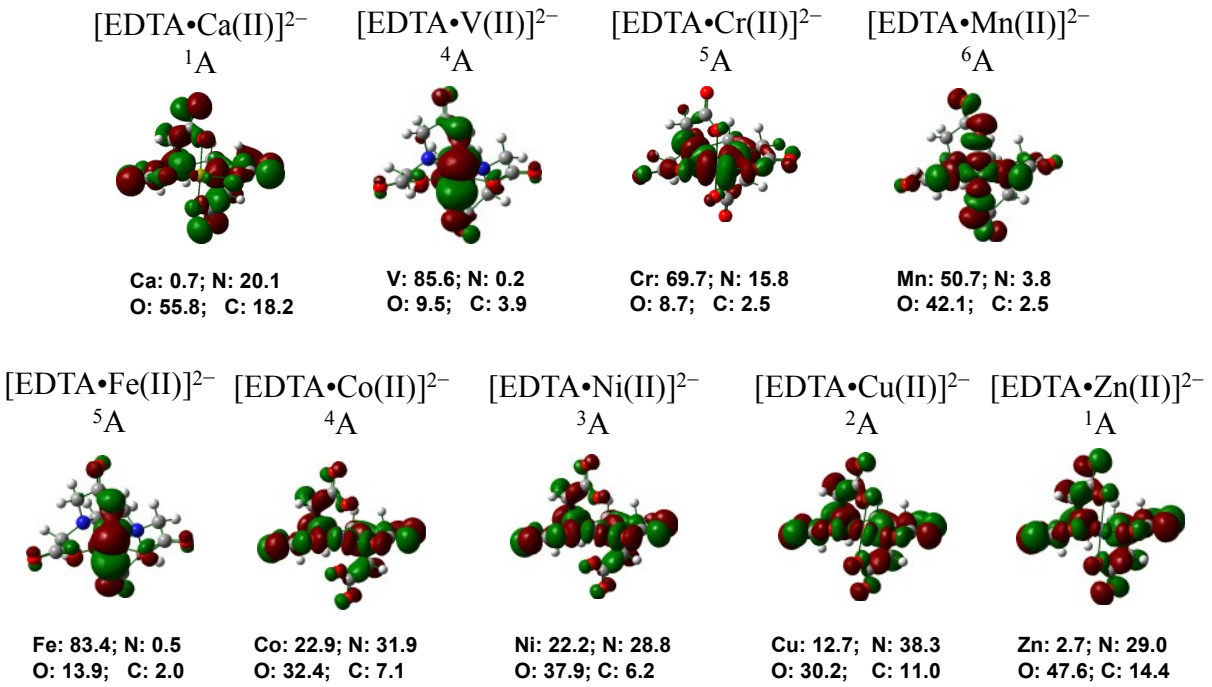

Fig. S2 Atom contribution (%) of the *M*, N, O and C in the HOMO pictures of the most stable isomers of [EDTA•*M*(II)]$^{2-}$ (*M* = Ca, V−Zn).

Cartesian coordinates for optimized isomers at the MN12SX/6-311+G(d,p) level.

Cluster: $[EDTA•Ca]^{2-}$: iso A (^1A)

N	-1.49938100	-0.02495500	0.82561400
C	-2.53990900	0.94980500	0.50951000
H	-2.09889800	1.95487500	0.57426000
H	-3.39307600	0.90063300	1.21164600
C	-3.06979200	0.80943000	-0.94337300
O	-4.23037900	1.16684600	-1.15038800
O	-2.22899200	0.37292300	-1.78507600
C	-2.04261200	-1.37709100	0.93984400
H	-2.36379200	-1.59943800	1.97439000
N	1.49944200	0.02500000	0.82552200
C	2.54004300	-0.94969100	0.50953700
H	2.09927900	-1.95485000	0.57453600
H	3.39331600	-0.90019300	1.21152100
C	3.06985800	-0.80929700	-0.94336200
O	4.23013000	-1.16766200	-1.15054800
O	2.22923100	-0.37224600	-1.78495000
C	2.04265000	1.37719200	0.93937500
H	2.36406400	1.59963400	1.97381800
H	2.94097600	1.43497100	0.30777300
C	1.12002000	2.51324600	0.43325900

O	0.29770300	2.18053300	-0.46671500
O	1.30043700	3.63144200	0.92193500
C	-0.68105600	0.34808200	1.97153200
H	-0.53809800	1.43588300	1.95327700
H	-1.19394700	0.10802600	2.92761900
C	0.68125400	-0.34779900	1.97159800
H	1.19419100	-0.10745800	2.92758700
H	0.53836100	-1.43561400	1.95365900
C	-1.12039100	-2.51335800	0.43338400
O	-1.30072000	-3.63149100	0.92223500
O	-0.29760200	-2.18056000	-0.46612600
H	-2.94110800	-1.43480400	0.30849000
Ca	-0.00002800	-0.00016900	-1.23536400

Cluster: $[EDTA•Ca]^{2-}$: iso B (^1A)

N	-1.34784600	-0.08686100	0.37580100
C	-1.71557800	1.15135800	-0.32682100
H	-2.31743400	0.86241300	-1.20059700
H	-0.80965400	1.63378100	-0.73407500
C	-2.51707200	2.24692200	0.45837500
O	-2.40917200	3.38994800	-0.02017300
O	-3.16926300	1.84925000	1.44166200
C	-2.43683000	-1.06278600	0.38253200

H	-2.20552800	-1.83303900	1.13402700
N	1.46362800	0.63998700	0.62723100
C	2.48638000	-0.20474200	1.25157500
H	2.82256400	0.21819700	2.21456400
H	3.36206100	-0.21686900	0.58391800
C	2.11705200	-1.69435300	1.44506700
O	2.60766300	-2.27674200	2.40810000
O	1.38640500	-2.18968000	0.52975800
C	2.09471500	1.73121400	-0.11512100
H	1.33211100	2.48906100	-0.34666900
H	2.88828300	2.23615400	0.46384300
C	2.67763100	1.27697200	-1.47810800
O	2.06240400	0.30885800	-2.03152900
O	3.63429300	1.90395000	-1.92264700
C	-0.74165900	0.13224700	1.69197500
H	-1.46680600	0.55088800	2.40790900
H	-0.40404600	-0.84621200	2.06427100
C	0.44447400	1.08616900	1.59106700
H	0.07739200	2.07368700	1.28454800
H	0.88428700	1.21418800	2.59693000
C	-2.59036700	-1.81655600	-0.96368700
O	-3.64218200	-2.41842700	-1.15461000
O	-1.57748400	-1.77957600	-1.74283800

H	-3.39570400	-0.60894400	0.67101300
Ca	0.41841100	-0.95122500	-1.09219100

Cluster: $[EDTA•Ca]^{2-}$: iso C (^1A)

N	0.00000000	1.42039500	-0.40848900
C	-1.43221500	1.66316800	-0.19202000
H	-1.53853800	2.20522800	0.76332100
H	-1.95921300	0.69724500	-0.07227200
C	-2.25865000	2.48759600	-1.25369700
O	-3.47432600	2.50121900	-1.00908900
O	-1.60300500	3.01621600	-2.16483000
C	0.79629000	2.63000200	-0.19285200
H	1.77659300	2.49084000	-0.67067700
N	0.00000000	-1.42039500	-0.40848900
C	1.43221500	-1.66316800	-0.19202000
H	1.95921300	-0.69724500	-0.07227200
C	2.25865000	-2.48759600	-1.25369700
O	3.47432600	-2.50121900	-1.00908900
O	1.60300500	-3.01621600	-2.16483000
C	-0.79629000	-2.63000200	-0.19285200
H	-1.77659300	-2.49084000	-0.67067700
H	-0.34026100	-3.51227700	-0.66328100
C	-1.09173800	-2.92601200	1.29875000

O	-0.84426900	-1.97399700	2.12433600
O	-1.56790700	-4.01851200	1.57286100
C	0.29560800	0.70328800	-1.65635600
H	-0.07541700	1.25413800	-2.53336900
H	1.38917200	0.63929000	-1.74213300
C	-0.29560800	-0.70328800	-1.65635600
H	-1.38917200	-0.63929000	-1.74213300
H	0.07541700	-1.25413800	-2.53336900
C	1.09173800	2.92601200	1.29875000
O	1.56790700	4.01851200	1.57286100
O	0.84426900	1.97399700	2.12433600
H	0.34026100	3.51227700	-0.66328100
H	1.53853800	-2.20522800	0.76332100
Ca	0.00000000	0.00000000	1.55686700

Cluster: $[EDTA•V]^{2-}$: iso B (^4A)

N	-1.29960100	-0.08374400	0.32068100
C	-1.94760000	1.02469100	-0.40657000
H	-2.35856900	0.60442900	-1.33519500
H	-1.17616500	1.74646500	-0.72501300
C	-3.09295900	1.82167700	0.30678300
O	-3.33455800	2.91923100	-0.22454500
O	-3.62815000	1.27011700	1.28611700

C	-2.07749800	-1.32606700	0.25441600
H	-1.64889400	-2.03095500	0.98152200
N	1.41936300	0.82786800	0.66667700
C	2.38343300	-0.00713400	1.39236100
H	2.65718900	0.43492700	2.36500800
H	3.29807600	-0.06729100	0.78472600
C	1.91204500	-1.46400500	1.57889200
O	2.37296000	-2.10392700	2.51840600
O	1.10489900	-1.86617500	0.68185100
C	2.09231200	1.85129200	-0.13091800
H	1.33568600	2.56609400	-0.48893100
H	2.84589200	2.41998200	0.44022500
C	2.75387100	1.23577300	-1.39502500
O	2.21249800	0.16417900	-1.81867600
O	3.69620900	1.84709600	-1.88775700
C	-0.81953200	0.30284200	1.65585600
H	-1.62769000	0.73971700	2.26026000
H	-0.46164000	-0.60672800	2.15240500
C	0.32212600	1.31424600	1.52681000
H	-0.06820200	2.24204400	1.09015000
H	0.69823800	1.56983500	2.53342600
C	-1.93151000	-1.99626400	-1.13677500
O	-2.79806200	-2.78749600	-1.48641700

O	-0.87627400	-1.68056000	-1.79508500
H	-3.13682300	-1.16831300	0.49665000
V	0.48870700	-0.53483000	-0.76229900

Cluster: $[EDTA•V]^{2-}$: iso C (^4A)

N	-0.57632600	1.36772900	-0.16033100
C	-2.05331600	1.41561000	-0.25704400
H	-2.44003400	1.69823100	0.73371000
H	-2.42774500	0.39869300	-0.43509700
C	-2.68254700	2.38237500	-1.31600600
O	-3.91999300	2.44549200	-1.24222400
O	-1.88906900	2.95592800	-2.08440700
C	0.00000000	2.69425600	0.13808300
H	0.31630800	3.21257000	-0.77405100
N	0.57632600	-1.36772900	-0.16033100
C	2.05331600	-1.41561000	-0.25704400
H	2.42774500	-0.39869300	-0.43509700
C	2.68254700	-2.38237500	-1.31600600
O	3.91999300	-2.44549200	-1.24222400
O	1.88906900	-2.95592800	-2.08440700
C	0.00000000	-2.69425600	0.13808300
H	-0.31630800	-3.21257000	-0.77405100
H	0.78487800	-3.32689800	0.57388000

C	-1.14019300	-2.63063300	1.16597900
O	-1.24879700	-1.50850200	1.79814400
O	-1.81993500	-3.62450000	1.35575000
C	0.06739200	0.75741400	-1.34884200
H	-0.35430700	1.19098700	-2.26634800
H	1.13102500	1.03119200	-1.30894800
C	-0.06739200	-0.75741400	-1.34884200
H	-1.13102500	-1.03119200	-1.30894800
H	0.35430700	-1.19098700	-2.26634800
C	1.14019300	2.63063300	1.16597900
O	1.81993500	3.62450000	1.35575000
O	1.24879700	1.50850200	1.79814400
H	-0.78487800	3.32689800	0.57388000
H	2.44003400	-1.69823100	0.73371000
V	0.00000000	0.00000000	1.36417900

Cluster: $[EDTA•Cr]^{2-}$: iso A (^5A)

N	1.46277200	0.04197300	0.98100600
C	2.50286000	-0.89623000	0.60532300
H	2.10621600	-1.91615000	0.70949100
H	3.41302300	-0.81226900	1.22962100
C	2.89247000	-0.73627100	-0.88202900
O	4.02839100	-1.07411400	-1.21514600

O	1.97217300	-0.27991500	-1.62389800
C	1.90732000	1.42779000	0.99218700
H	2.08821500	1.79114900	2.02063600
N	-1.46255000	-0.04163400	0.98129200
C	-2.50272700	0.89646600	0.60557500
H	-2.10610500	1.91641200	0.70953000
H	-3.41280600	0.81257800	1.23001200
C	-2.89248000	0.73642700	-0.88172800
O	-4.02884900	1.07308200	-1.21451500
O	-1.97243600	0.27951200	-1.62356600
C	-1.90704800	-1.42746200	0.99290300
H	-2.08791000	-1.79050000	2.02146500
H	-2.86884600	-1.48862400	0.46330400
C	-0.98543700	-2.44623400	0.27658800
O	-0.24347100	-1.99400400	-0.64794400
O	-1.07822800	-3.61921100	0.64133600
C	0.68605200	-0.33540100	2.13899400
H	0.55730200	-1.42712000	2.12693300
H	1.20354100	-0.08225400	3.09171000
C	-0.68564300	0.33601600	2.13905700
H	-1.20295900	0.08306600	3.09191900
H	-0.55692000	1.42773500	2.12673800
C	0.98593600	2.44643400	0.27539300

O	1.07777900	3.61928600	0.64077700
O	0.24344300	1.99389700	-0.64856900
H	2.86911700	1.48871500	0.46257400
Cr	-0.00006900	-0.00010700	-1.04422500

Cluster: $[EDTA•Cr]^{2-}$: iso B (^5A)

N	1.27585000	0.09236900	0.32025500
C	2.00826400	-1.00177800	-0.35697600
H	2.35397000	-0.60716400	-1.32226800
H	1.30155600	-1.80635200	-0.61008200
C	3.23426000	-1.63762800	0.38363000
O	3.60559900	-2.71147600	-0.12029000
O	3.69247100	-1.00864800	1.35568000
C	1.98759000	1.37610000	0.21792200
H	1.50972200	2.08127500	0.91337400
N	-1.38608500	-0.84721100	0.64555600
C	-2.41884000	-0.07605400	1.35840400
H	-2.71393300	-0.58266600	2.29136400
H	-3.30556300	-0.02763200	0.71019400
C	-2.02317400	1.39561700	1.64062200
O	-2.55442600	1.93057000	2.61452400
O	-1.22479700	1.89098100	0.79870900
C	-1.98896700	-1.89141300	-0.18920600

H	-1.18638600	-2.55250700	-0.55040200
H	-2.72115400	-2.50750100	0.35821300
C	-2.65106000	-1.26923100	-1.44561600
O	-2.12277500	-0.17519600	-1.83287200
O	-3.57583400	-1.88021100	-1.96706600
C	0.81086400	-0.27533900	1.66917600
H	1.63385200	-0.67646100	2.27672300
H	0.42651800	0.63399600	2.14439200
C	-0.30649900	-1.31002600	1.54641000
H	0.10231900	-2.24307100	1.13994600
H	-0.71029600	-1.54506200	2.54548600
C	1.81094700	1.97717900	-1.19590000
O	2.62808900	2.79590700	-1.58969000
O	0.76717700	1.57749100	-1.83484900
H	3.04960200	1.27975500	0.47466100
Cr	-0.47803800	0.44822500	-0.76234300

Cluster: $[EDTA•Cr]^{2-}$: iso C (^5A)

N	-0.50898100	1.32006200	-0.37717400
C	-1.99205300	1.29446400	-0.36575100
H	-2.31740300	1.69178900	0.60639700
H	-2.33117900	0.24792900	-0.39167700
C	-2.74981400	2.08394900	-1.49255300

O	-3.97268200	1.88206600	-1.47780700
O	-2.05479800	2.80268200	-2.23254000
C	0.00000000	2.63405500	0.04634400
H	1.05414500	2.71450500	-0.25725500
N	0.50898100	-1.32006200	-0.37717400
C	1.99205300	-1.29446400	-0.36575100
H	2.33117900	-0.24792900	-0.39167700
C	2.74981400	-2.08394900	-1.49255300
O	3.97268200	-1.88206600	-1.47780700
O	2.05479800	-2.80268200	-2.23254000
C	0.00000000	-2.63405500	0.04634400
H	-1.05414500	-2.71450500	-0.25725500
H	0.54754100	-3.45877000	-0.42551600
C	0.02690400	-2.75980200	1.58698600
O	0.10958600	-1.64278400	2.22982700
O	-0.07155000	-3.86765600	2.08482400
C	0.06195400	0.76110600	-1.62367500
H	-0.42936500	1.19562700	-2.50381800
H	1.12123200	1.04685400	-1.65716100
C	-0.06195400	-0.76110600	-1.62367500
H	-1.12123200	-1.04685400	-1.65716100
H	0.42936500	-1.19562700	-2.50381800
C	-0.02690400	2.75980200	1.58698600

O	0.07155000	3.86765600	2.08482400
O	-0.10958600	1.64278400	2.22982700
H	-0.54754100	3.45877000	-0.42551600
H	2.31740300	-1.69178900	0.60639700
Cr	0.00000000	0.00000000	1.12722700

Cluster: $[EDTA•Mn]^{2-}$: iso A (^6A)

N	-1.47353600	-0.00443400	0.89610400
C	-2.46311300	0.98618100	0.49033300
H	-2.01969900	1.98496300	0.59688700
H	-3.38554700	0.94172000	1.09711300
C	-2.83557100	0.84123500	-1.00805800
O	-3.95348400	1.22592000	-1.34886100
O	-1.92633600	0.35662600	-1.75034000
C	-2.03225500	-1.34978500	0.97594400
H	-2.35501400	-1.59790900	2.00343300
N	1.47360800	0.00459700	0.89600500
C	2.46315600	-0.98609100	0.49034100
H	2.01975200	-1.98485400	0.59711300
H	3.38563700	-0.94151500	1.09704000
C	2.83549500	-0.84142100	-1.00810600
O	3.95340000	-1.22612700	-1.34891500
O	1.92620700	-0.35694000	-1.75040600

C	2.03233200	1.34996200	0.97556400
H	2.35513900	1.59827900	2.00299100
H	2.92875400	1.38690500	0.34042600
C	1.10690800	2.46894200	0.44324300
O	0.25173700	2.09946900	-0.40960600
O	1.30751100	3.60745700	0.87431500
C	-0.67900300	0.35454900	2.05946700
H	-0.52656100	1.44131200	2.05058000
H	-1.20494800	0.10727500	3.00583700
C	0.67915500	-0.35417500	2.05948800
H	1.20516400	-0.10672500	3.00577700
H	0.52671800	-1.44094000	2.05080900
C	-1.10684700	-2.46886200	0.44379700
O	-1.30749000	-3.60731500	0.87501500
O	-0.25177000	-2.09955600	-0.40921700
H	-2.92870400	-1.38684900	0.34085200
Mn	-0.00003700	-0.00009100	-0.96486400

Cluster: $[EDTA•Mn]^{2-}$: iso B (^{6}A)

N	1.29273600	0.11253800	0.37859200
C	1.86065700	-1.03137800	-0.35911900
H	2.33146200	-0.62559200	-1.26620500
H	1.04419100	-1.67687300	-0.71841700

C	2.91397200	-1.93260400	0.37002300
O	3.04887600	-3.05805100	-0.14200700
O	3.49586100	-1.42527200	1.34794900
C	2.17984100	1.27475400	0.35842600
H	1.85577600	1.97115700	1.14619700
N	-1.36504400	-0.87715000	0.66428900
C	-2.44658700	-0.14249500	1.31936500
H	-2.73287800	-0.60706300	2.27862700
H	-3.32881900	-0.18606100	0.66250400
C	-2.18775700	1.36491600	1.53861700
O	-2.75732200	1.90450400	2.48146800
O	-1.44407600	1.91874700	0.66676400
C	-1.88536100	-1.92873800	-0.20040300
H	-1.07024100	-2.62112700	-0.45370600
H	-2.68304400	-2.52391600	0.27717400
C	-2.41038300	-1.36905500	-1.54331600
O	-1.86837800	-0.27978900	-1.92731700
O	-3.25895600	-2.02201300	-2.13928900
C	0.78663600	-0.23273700	1.70954700
H	1.58838600	-0.60373200	2.36520500
H	0.36530900	0.68481100	2.14446600
C	-0.30567000	-1.29029100	1.59212300
H	0.13749000	-2.22696400	1.23171500

H	-0.71773100	-1.50009100	2.59561900
C	2.07700100	2.06156300	-0.96932300
O	2.98873200	2.82613200	-1.25713300
O	1.00400200	1.87215300	-1.64554000
H	3.22399400	1.00244900	0.56192900
Mn	-0.50686900	0.78921500	-0.80400300

Cluster: $[EDTA•Mn]^{2-}$: iso C (^6A)

N	-0.60407500	1.39430200	-0.19274200
C	-2.07050800	1.48791000	-0.36376800
H	-2.50306200	1.78235000	0.60342800
H	-2.46982500	0.48608500	-0.57080600
C	-2.61398500	2.47219100	-1.45348200
O	-3.85309800	2.55000400	-1.46161300
O	-1.76349700	3.04285000	-2.15993300
C	0.00000000	2.69364900	0.15401500
H	0.40838400	3.19924100	-0.72807200
N	0.60407500	-1.39430200	-0.19274200
C	2.07050800	-1.48791000	-0.36376800
H	2.46982500	-0.48608500	-0.57080600
C	2.61398500	-2.47219100	-1.45348200
O	3.85309800	-2.55000400	-1.46161300
O	1.76349700	-3.04285000	-2.15993300

C	0.00000000	-2.69364900	0.15401500
H	-0.40838400	-3.19924100	-0.72807200
H	0.79046700	-3.35884800	0.52619000
C	-1.06448100	-2.62442800	1.26629900
O	-1.11046100	-1.52964100	1.95340900
O	-1.75561100	-3.60844200	1.46357900
C	0.07112000	0.75956300	-1.35078200
H	-0.31717800	1.18570900	-2.28649300
H	1.13568400	1.02627500	-1.28910400
C	-0.07112000	-0.75956300	-1.35078200
H	-1.13568400	-1.02627500	-1.28910400
H	0.31717800	-1.18570900	-2.28649300
C	1.06448100	2.62442800	1.26629900
O	1.75561100	3.60844200	1.46357900
O	1.11046100	1.52964100	1.95340900
H	-0.79046700	3.35884800	0.52619000
H	2.50306200	-1.78235000	0.60342800
Mn	0.00000000	0.00000000	1.37734700

Cluster: $[EDTA•Fe]^{2-}$: iso A (^5A)

N	-1.45065900	0.00571700	0.88848200
C	-2.44025200	0.99899800	0.48710300
H	-1.99794500	1.99777300	0.59956100

H	-3.36623300	0.94809600	1.08708800
C	-2.78538900	0.84602400	-1.01245600
O	-3.88834400	1.23492100	-1.39065800
O	-1.85930100	0.33792500	-1.71820000
C	-2.01735500	-1.34142800	0.96463100
H	-2.34683800	-1.58154800	1.99107100
N	1.45059800	-0.00606700	0.88852000
C	2.44023600	-0.99913800	0.48675600
H	1.99799500	-1.99801000	0.59876200
H	3.36620700	-0.94846300	1.08674900
C	2.78534100	-0.84544000	-1.01271700
O	3.88836400	-1.23409000	-1.39100900
O	1.85919400	-0.33722500	-1.71828800
C	2.01729400	1.34102300	0.96517400
H	2.34657400	1.58093900	1.99172200
H	2.90920600	1.37106300	0.32360700
C	1.09796000	2.47186900	0.43949700
O	0.28671500	2.13315800	-0.46259800
O	1.27518900	3.59386600	0.92683800
C	-0.67342500	0.36025700	2.06540300
H	-0.51131300	1.44593300	2.05813300
H	-1.21505600	0.11589000	3.00243200
C	0.67332500	-0.36107700	2.06524500

H	1.21488400	-0.11710400	3.00240700
H	0.51119500	-1.44674800	2.05752400
C	-1.09778100	-2.47205900	0.43895900
O	-1.27465200	-3.59407900	0.92639500
O	-0.28670800	-2.13316100	-0.46321100
H	-2.90906300	-1.37138500	0.32279100
Fe	-0.00009900	0.00005100	-0.90617700

Cluster: $[EDTA•Fe]^{2-}$: iso B (^5A)

N	1.27881400	0.09823800	0.35849300
C	1.92456600	-1.00279600	-0.38362500
H	2.34161800	-0.56740400	-1.30277900
H	1.15589700	-1.71158000	-0.72216800
C	3.06144300	-1.81525400	0.32230900
O	3.30346200	-2.90451200	-0.22732000
O	3.59490200	-1.28874400	1.31797300
C	2.10933800	1.30366800	0.36166400
H	1.73680600	1.97984000	1.14541900
N	-1.35295200	-0.92776700	0.65505400
C	-2.42116700	-0.22283500	1.36207300
H	-2.67012300	-0.71210500	2.31918900
H	-3.32530100	-0.25618600	0.73547800
C	-2.15028100	1.27822700	1.60373000

O	-2.69321500	1.80281600	2.57250100
O	-1.42877400	1.83875700	0.72212400
C	-1.87936000	-1.94836400	-0.23831000
H	-1.05602000	-2.60342600	-0.55691900
H	-2.64670900	-2.58747600	0.23242600
C	-2.46121700	-1.32339500	-1.52494300
O	-1.96498700	-0.18994000	-1.84377700
O	-3.30574000	-1.95684300	-2.14467400
C	0.80015300	-0.29508000	1.68716200
H	1.62094500	-0.66921100	2.31639500
H	0.36899800	0.59965000	2.15628900
C	-0.27431000	-1.36523600	1.54711900
H	0.17490300	-2.27982700	1.14110800
H	-0.66767300	-1.62230800	2.54694500
C	1.97125200	2.07342700	-0.96764300
O	2.83777600	2.87784400	-1.27828400
O	0.90198600	1.81647700	-1.63197000
H	3.16294000	1.08299500	0.57595200
Fe	-0.52781200	0.73433500	-0.77661400

Cluster: $[EDTA•Fe]^{2-}$: iso C (^5A)

N	1.48231400	0.12183600	0.21693700
C	2.23891900	-1.14180600	0.35707200
H	2.68877400	-1.37126600	-0.61917300

H	1.53428900	-1.96034200	0.55436300
C	3.37358400	-1.18966500	1.43573800
O	3.98357200	-2.27106400	1.44826000
O	3.52911300	-0.16689600	2.12761400
C	2.35892800	1.25309600	-0.13105400
H	2.60456200	1.86341600	0.74512600
N	-1.48204000	-0.12212000	0.21733800
C	-2.23907900	1.14127000	0.35751800
H	-1.53470000	1.96003400	0.55476800
C	-3.37366300	1.18866000	1.43632300
O	-3.98391200	2.26990500	1.44912300
O	-3.52888000	0.16570200	2.12798700
C	-2.35828100	-1.25367900	-0.13066700
H	-2.60235900	-1.86503000	0.74523000
H	-3.32177200	-0.86276400	-0.48246300
C	-1.80591000	-2.13714400	-1.25974700
O	-0.80481200	-1.65049100	-1.92411100
O	-2.35266100	-3.19836500	-1.49764400
C	0.63957600	0.41185700	1.40022300
H	1.21543900	0.24153500	2.32039200
H	0.38593100	1.48045200	1.36749800
C	-0.63905700	-0.41160400	1.40057200
H	-0.38544900	-1.48020800	1.36839000
H	-1.21468400	-0.24080400	2.32079400

C	1.80582100	2.13788300	-1.25869800
O	2.35242200	3.19935400	-1.49579800
O	0.80423400	1.65197600	-1.92289000
H	3.32164500	0.86171700	-0.48449000
H	-2.68911200	1.37059000	-0.61867900
Fe	-0.00008200	0.00040300	-1.34444900

Cluster: $[EDTA•Co]^{2-}$: iso A (^4A)

N	-1.48276300	0.01814000	0.89289200
C	-2.44487800	1.02069400	0.45217200
H	-2.00542300	2.01622400	0.58820800
H	-3.39801100	0.97024600	1.00750600
C	-2.73440400	0.87228600	-1.06652400
O	-3.82248300	1.28474900	-1.46939800
O	-1.80493300	0.34841200	-1.75170900
C	-2.06568600	-1.31585200	0.96338100
H	-2.42200000	-1.55458600	1.98162300
N	1.48296900	-0.01798200	0.89289300
C	2.44527000	-1.02035400	0.45225200
H	2.00588600	-2.01596500	0.58806400
H	3.39828200	-0.96991200	1.00779200
C	2.73496800	-0.87162300	-1.06643600
O	3.82341600	-1.28325400	-1.46916600

O	1.80517100	-0.34848200	-1.75169100
C	2.06552200	1.31616700	0.96311500
H	2.42211400	1.55506400	1.98123100
H	2.94140000	1.34443900	0.30022000
C	1.13134600	2.43768200	0.46349500
O	0.21725900	2.05687500	-0.32033500
O	1.36998400	3.58317600	0.85323800
C	-0.67950000	0.35883200	2.05961900
H	-0.52281700	1.44412500	2.06307200
H	-1.20485100	0.10144300	3.00277200
C	0.67976200	-0.35861300	2.05963400
H	1.20513500	-0.10125900	3.00278900
H	0.52297700	-1.44390000	2.06308600
C	-1.13196500	-2.43775900	0.46385500
O	-1.37110900	-3.58313000	0.85355000
O	-0.21758700	-2.05743500	-0.31994800
H	-2.94178200	-1.34398400	0.30078200
Co	-0.00010000	-0.00070700	-0.80930900

Cluster: $[EDTA•Co]^{2-}$: iso B (^4A)

N	-1.24402100	-0.11773700	0.36924900
C	-1.89860800	1.00143700	-0.34042300
H	-2.31413800	0.58911800	-1.27103400

H	-1.13671600	1.72661100	-0.65747000
C	-3.04024300	1.77852100	0.39800900
O	-3.28591800	2.88852100	-0.10546800
O	-3.57131400	1.20796800	1.37013600
C	-2.06165200	-1.33898100	0.32324900
H	-1.71689600	-2.01440700	1.11996400
N	1.35682900	0.93233900	0.66688100
C	2.47782000	0.24182600	1.29648100
H	2.78578900	0.72653500	2.23878300
H	3.33421700	0.29021200	0.60699300
C	2.23524000	-1.26163700	1.53645300
O	2.82877800	-1.79933700	2.46570900
O	1.46676300	-1.81535600	0.68715300
C	1.80774700	1.98792200	-0.23045700
H	0.96959100	2.66724400	-0.43854000
H	2.62513200	2.59521300	0.19432000
C	2.25040400	1.41816200	-1.59683700
O	1.69319800	0.32103400	-1.92527200
O	3.04881200	2.07137600	-2.25906300
C	-0.77344500	0.23349700	1.71526000
H	-1.59966100	0.58183600	2.35115600
H	-0.34171300	-0.67616700	2.15382900
C	0.30020300	1.31124000	1.61359500

H	-0.16022500	2.24792100	1.27557400
H	0.71874500	1.50585600	2.61673900
C	-1.87690400	-2.11642400	-1.00064500
O	-2.75790000	-2.90200800	-1.32808100
O	-0.77880100	-1.90509400	-1.62491200
H	-3.12189500	-1.12224000	0.50151600
Co	0.49984400	-0.69963500	-0.68423900

Cluster: $[EDTA•Co]^{2-}$: iso C (^4A)

N	-0.58103500	1.33928500	-0.21923600
C	-2.05663900	1.39905700	-0.32300200
H	-2.45366000	1.65025000	0.67119200
H	-2.43807200	0.39453500	-0.54637800
C	-2.66724800	2.40660600	-1.35599000
O	-3.90596400	2.46463200	-1.30140700
O	-1.86183300	3.01029400	-2.08756000
C	0.00000000	2.64684500	0.13088100
H	0.34476500	3.19007100	-0.75564800
N	0.58103500	-1.33928500	-0.21923600
C	2.05663900	-1.39905700	-0.32300200
H	2.43807200	-0.39453500	-0.54637800
C	2.66724800	-2.40660600	-1.35599000
O	3.90596400	-2.46463200	-1.30140700

O	1.86183300	-3.01029400	-2.08756000
C	0.00000000	-2.64684500	0.13088100
H	-0.34476500	-3.19007100	-0.75564800
H	0.78641900	-3.27522000	0.56982000
C	-1.11641600	-2.54511400	1.17906300
O	-1.17967200	-1.42237400	1.81764700
O	-1.82718600	-3.51300300	1.38454100
C	0.05582000	0.75748300	-1.42034700
H	-0.38488500	1.19148400	-2.32827900
H	1.11516600	1.04742800	-1.39589500
C	-0.05582000	-0.75748300	-1.42034700
H	-1.11516600	-1.04742800	-1.39589500
H	0.38488500	-1.19148400	-2.32827900
C	1.11641600	2.54511400	1.17906300
O	1.82718600	3.51300300	1.38454100
O	1.17967200	1.42237400	1.81764700
H	-0.78641900	3.27522000	0.56982000
H	2.45366000	-1.65025000	0.67119200
Co	0.00000000	0.00000000	1.30003300

Cluster: $[EDTA•Ni]^{2-}$: iso A (^3A)

N	1.44720000	-0.04564200	0.88749200
C	2.40133400	-1.05729000	0.43845800

H	1.95265700	-2.04931900	0.56899600
H	3.35319600	-1.01290000	0.99478000
C	2.67880900	-0.88696200	-1.08057700
O	3.75699000	-1.31377300	-1.49850700
O	1.75308100	-0.32905900	-1.73656300
C	2.05096900	1.28649300	0.95254000
H	2.39125600	1.52419900	1.97502600
N	-1.44723300	0.04554000	0.88746900
C	-2.40138700	1.05722700	0.43855200
H	-1.95274100	2.04925000	0.56924000
H	-3.35326100	1.01273200	0.99484500
C	-2.67882300	0.88710900	-1.08051200
O	-3.75700400	1.31395500	-1.49840600
O	-1.75306400	0.32933400	-1.73656400
C	-2.05097100	-1.28661900	0.95235500
H	-2.39131700	-1.52439900	1.97480400
H	-2.93814600	-1.29121400	0.30484900
C	-1.14670100	-2.42131900	0.42458000
O	-0.25802300	-2.05787100	-0.39283300
O	-1.39182700	-3.56159300	0.82855400
C	0.66729700	-0.37697800	2.07453000
H	0.48238200	-1.45862700	2.07176900
H	1.21899000	-0.13750400	3.00524400

C	-0.66736300	0.37673900	2.07456700
H	-1.21907400	0.13713200	3.00523400
H	-0.48245800	1.45838900	2.07196000
C	1.14676200	2.42123600	0.42475800
O	1.39193900	3.56150600	0.82871700
O	0.25806700	2.05780300	-0.39264000
H	2.93818200	1.29110400	0.30508600
Ni	-0.00001000	0.00005800	-0.68557600

Cluster: $[EDTA•Ni]^{2-}$: iso B (^3A)

N	1.26696300	0.10343900	0.34298500
C	1.94145900	-0.99611000	-0.37696600
H	2.29545200	-0.58470300	-1.33204600
H	1.20097800	-1.76469600	-0.64426000
C	3.14884000	-1.70819200	0.32354000
O	3.43571100	-2.80345200	-0.18938100
O	3.68062700	-1.10711900	1.27588000
C	1.99823900	1.36928100	0.22871600
H	1.59450800	2.06606200	0.97648800
N	-1.34325600	-0.88611300	0.70647300
C	-2.35842700	-0.08109300	1.39108000
H	-2.63418800	-0.51898000	2.36447800
H	-3.26139500	-0.06969500	0.76354600

C	-1.95437400	1.39617600	1.57095300
O	-2.47161600	2.02129700	2.49188400
O	-1.13980800	1.82996300	0.69879400
C	-1.94939000	-1.93472200	-0.10765600
H	-1.16787800	-2.64858200	-0.40503100
H	-2.72920100	-2.49807000	0.43114700
C	-2.54171800	-1.35095500	-1.41643300
O	-2.01413000	-0.26502200	-1.81007700
O	-3.42717600	-2.00083600	-1.96500100
C	0.84506400	-0.26803200	1.69844200
H	1.68763900	-0.65802000	2.28630300
H	0.46236000	0.63766600	2.18312400
C	-0.25964300	-1.31916100	1.60525000
H	0.16022000	-2.25443900	1.21550200
H	-0.65065900	-1.53880200	2.61383000
C	1.74942300	2.01851500	-1.15194300
O	2.55387400	2.85427900	-1.54652100
O	0.68805700	1.63968600	-1.75906300
H	3.07245100	1.23926100	0.40917900
Ni	-0.48776300	0.49882500	-0.65608800

Cluster: $[EDTA•Ni]^{2-}$: iso C (^3A)

N	-0.59691300	1.33047000	-0.18620900

C	-2.06971000	1.40881400	-0.30727900
H	-2.47240300	1.65108500	0.68546300
H	-2.45660300	0.40988300	-0.54394500
C	-2.65266700	2.43366600	-1.33765400
O	-3.88917500	2.52400700	-1.28113900
O	-1.83447800	3.01685400	-2.07250200
C	0.00000000	2.62714400	0.18276000
H	0.28049500	3.20754100	-0.70298300
N	0.59691300	-1.33047000	-0.18620900
C	2.06971000	-1.40881400	-0.30727900
H	2.45660300	-0.40988300	-0.54394500
C	2.65266700	-2.43366600	-1.33765400
O	3.88917500	-2.52400700	-1.28113900
O	1.83447800	-3.01685400	-2.07250200
C	0.00000000	-2.62714400	0.18276000
H	-0.28049500	-3.20754100	-0.70298300
H	0.76134100	-3.22461900	0.70205300
C	-1.18273600	-2.47618100	1.14908100
O	-1.29446900	-1.32123000	1.71356200
O	-1.89896100	-3.44015100	1.36025800
C	0.05271000	0.75731700	-1.38879600
H	-0.38830400	1.19567200	-2.29368100
H	1.11025200	1.05321500	-1.35658900

C	-0.05271000	-0.75731700	-1.38879600
H	-1.11025200	-1.05321500	-1.35658900
H	0.38830400	-1.19567200	-2.29368100
C	1.18273600	2.47618100	1.14908100
O	1.89896100	3.44015100	1.36025800
O	1.29446900	1.32123000	1.71356200
H	-0.76134100	3.22461900	0.70205300
H	2.47240300	-1.65108500	0.68546300
Ni	0.00000000	0.00000000	1.23307400

Cluster: $[EDTA•Cu]^{2-}$: iso A (^2A)

N	-1.45913700	-0.04493500	1.01920200
C	-2.47854400	0.89002200	0.59536600
H	-2.08925400	1.91102500	0.70642000
H	-3.41586700	0.80897300	1.17841500
C	-2.81650300	0.71430000	-0.90409800
O	-3.93756100	1.06719600	-1.27409600
O	-1.89323000	0.22215500	-1.61670400
C	-1.89123100	-1.42995500	1.01415700
H	-2.07940500	-1.80624100	2.03671000
N	1.45907000	0.04500500	1.01929000
C	2.47848300	-0.88999100	0.59555700
H	2.08916100	-1.91098200	0.70661800

H	3.41576700	-0.80894400	1.17866700
C	2.81656100	-0.71430700	-0.90388600
O	3.93757600	-1.06739700	-1.27382600
O	1.89331800	-0.22224600	-1.61658900
C	1.89118300	1.43002000	1.01417700
H	2.07930000	1.80637300	2.03671600
H	2.84556200	1.49920800	0.47284700
C	0.94602200	2.42706900	0.30487600
O	0.16231600	1.95608200	-0.57458700
O	1.04889200	3.61027100	0.63380000
C	-0.68897600	0.33276300	2.17799200
H	-0.56663000	1.42516900	2.17125300
H	-1.20428400	0.07209700	3.12993200
C	0.68883800	-0.33261200	2.17805800
H	1.20408500	-0.07187900	3.13001300
H	0.56649500	-1.42501900	2.17139000
C	-0.94601200	-2.42703900	0.30498700
O	-1.04887200	-3.61021700	0.63400000
O	-0.16227000	-1.95610400	-0.57447200
H	-2.84557500	-1.49919500	0.47277100
Cu	0.00002900	-0.00002100	-0.91808600

Cluster: $[EDTA•Cu]^{2-}$: iso B (^2A)

N	1.25878900	0.10728400	0.33407700
C	2.01279200	-0.99990800	-0.29219400
H	2.32123500	-0.65740700	-1.28875800
H	1.33786200	-1.84841400	-0.46910700
C	3.28137300	-1.54007100	0.45666800
O	3.69148700	-2.61765300	-0.00677300
O	3.72627100	-0.84773300	1.39019100
C	1.93049500	1.40052000	0.14988400
H	1.46158900	2.12545000	0.82911900
N	-1.34367600	-0.84581600	0.70741900
C	-2.40097100	-0.05242300	1.35286700
H	-2.72790800	-0.53361300	2.28872100
H	-3.26119400	-0.02856600	0.66908300
C	-2.01894200	1.42879000	1.60845600
O	-2.58488300	1.97743600	2.55805400
O	-1.20241300	1.90706400	0.78174300
C	-1.91832300	-1.93928000	-0.07681700
H	-1.11789300	-2.64218900	-0.34901000
H	-2.68662600	-2.50007600	0.47914200
C	-2.51110300	-1.40109200	-1.40134200
O	-1.99585800	-0.31247200	-1.80965400
O	-3.38088900	-2.07085600	-1.94750300
C	0.82514900	-0.19240900	1.70719500

H	1.66856600	-0.54793800	2.31422200
H	0.43648700	0.73533300	2.13873900
C	-0.27947000	-1.24223700	1.65177200
H	0.13653200	-2.20066900	1.31889400
H	-0.69706000	-1.40467200	2.65907000
C	1.68304800	1.92443200	-1.27982300
O	2.44853800	2.75676800	-1.74385600
O	0.64379200	1.44701400	-1.86548200
H	3.00245300	1.33634500	0.36996800
Cu	-0.47146500	0.38281600	-0.70221800

Cluster: $[EDTA•Cu]^{2-}$: iso C (^2A)

N	-0.52156900	1.29623600	-0.40451800
C	-2.00426000	1.29785200	-0.41000300
H	-2.33318000	1.66753100	0.57060100
H	-2.36578100	0.26369200	-0.48161900
C	-2.72753800	2.14325500	-1.52043400
O	-3.95663700	1.98401200	-1.50749900
O	-2.00900500	2.85059000	-2.24869800
C	0.00000000	2.59648700	0.04150900
H	1.04020900	2.69553400	-0.29862100
N	0.52156900	-1.29623600	-0.40451800
C	2.00426000	-1.29785200	-0.41000300

H	2.36578100	-0.26369200	-0.48161900
C	2.72753800	-2.14325500	-1.52043400
O	3.95663700	-1.98401200	-1.50749900
O	2.00900500	-2.85059000	-2.24869800
C	0.00000000	-2.59648700	0.04150900
H	-1.04020900	-2.69553400	-0.29862100
H	0.56985900	-3.42797600	-0.38805400
C	-0.02613000	-2.67456400	1.58141300
O	0.04534700	-1.54523500	2.19252100
O	-0.15064600	-3.76830200	2.10770300
C	0.05314900	0.75897900	-1.65609400
H	-0.44910100	1.19829200	-2.52703700
H	1.10812300	1.05811700	-1.69321000
C	-0.05314900	-0.75897900	-1.65609400
H	-1.10812300	-1.05811700	-1.69321000
H	0.44910100	-1.19829200	-2.52703700
C	0.02613000	2.67456400	1.58141300
O	0.15064600	3.76830200	2.10770300
O	-0.04534700	1.54523500	2.19252100
H	-0.56985900	3.42797600	-0.38805400
H	2.33318000	-1.66753100	0.57060100
Cu	0.00000000	0.00000000	1.03993100

Cluster: $[EDTA•Zn]^{2-}$: iso A (^1A)

N	-1.46142900	0.01902900	0.93531300
C	-2.41893900	1.01986200	0.48833300
H	-1.97587900	2.01527900	0.61778200
H	-3.37212700	0.97876600	1.04468700
C	-2.71880200	0.87407700	-1.02563900
O	-3.81153800	1.27954000	-1.42001400
O	-1.79412900	0.35863400	-1.72642000
C	-2.03503100	-1.31900800	1.00030200
H	-2.35652000	-1.57572700	2.02558900
N	1.46138000	-0.01880500	0.93518500
C	2.41873100	-1.01982500	0.48829000
H	1.97548900	-2.01516600	0.61773800
H	3.37189200	-0.97888000	1.04469600
C	2.71877100	-0.87401400	-1.02564900
O	3.81117000	-1.28033300	-1.42008100
O	1.79400900	-0.35889700	-1.72654500
C	2.03521200	1.31915000	0.99990900
H	2.35661700	1.57609500	2.02517200
H	2.93401600	1.34076500	0.36771000
C	1.12268800	2.44294900	0.45615500
O	0.25179500	2.07842900	-0.37928000
O	1.34875900	3.58414800	0.87070700

C	-0.67417900	0.36498800	2.10458700
H	-0.50570300	1.44952000	2.09981400
H	-1.20796900	0.12064300	3.04671700
C	0.67417700	-0.36450700	2.10457900
H	1.20804500	-0.12004200	3.04663400
H	0.50565400	-1.44903400	2.09998200
C	-1.12208100	-2.44275200	0.45714500
O	-1.34875800	-3.58406000	0.87106400
O	-0.25166100	-2.07840000	-0.37885400
H	-2.93374800	-1.34098600	0.36798400
Zn	0.00000400	-0.00002700	-0.84368900

Cluster: $[EDTA•Zn]^{2-}$: iso B (^1A)

N	1.26931900	0.09728500	0.37744800
C	1.94399400	-0.98074500	-0.37287300
H	2.33742800	-0.53079200	-1.29535800
H	1.19786100	-1.71645300	-0.70350700
C	3.11273900	-1.75200900	0.32613200
O	3.38826000	-2.83313700	-0.22352600
O	3.63406600	-1.20639500	1.31796500
C	2.04966800	1.33632400	0.36643700
H	1.68704900	1.98202600	1.17966100
N	-1.32599400	-1.01151300	0.67826800

C	-2.42503700	-0.33272500	1.35297400
H	-2.68616000	-0.82035700	2.30776100
H	-3.31287400	-0.39381900	0.70565400
C	-2.21032200	1.17748000	1.60096500
O	-2.82060500	1.68320500	2.53762200
O	-1.45462800	1.77067600	0.76772400
C	-1.78845300	-2.01284400	-0.26712700
H	-0.94854000	-2.66828200	-0.53651600
H	-2.58914500	-2.65643200	0.13636300
C	-2.28103200	-1.37996300	-1.58988700
O	-1.77497300	-0.24838600	-1.88635400
O	-3.07952000	-2.02443900	-2.26015900
C	0.81268300	-0.31484700	1.70818200
H	1.64760700	-0.67311900	2.32682400
H	0.36602700	0.56771600	2.18600500
C	-0.24209100	-1.41096100	1.57662600
H	0.22838300	-2.32107900	1.18472200
H	-0.63032400	-1.66062800	2.58034800
C	1.84296600	2.14102100	-0.93817900
O	2.69392400	2.96866400	-1.23910400
O	0.76337500	1.89947100	-1.58338000
H	3.11778800	1.15090800	0.53390300
Zn	-0.52360900	0.70794200	-0.66738900

Cluster: $[EDTA•Zn]^{2-}$: iso C (^1A)

N	-0.61254600	1.35661600	-0.23932000
C	-2.07820200	1.46947500	-0.41849400
H	-2.51610000	1.73428000	0.55355100
H	-2.48148500	0.47791400	-0.66151500
C	-2.59663400	2.49216900	-1.48205400
O	-3.83542900	2.57289600	-1.51100400
O	-1.73323800	3.08692200	-2.15298300
C	0.00000000	2.63351000	0.16723100
H	0.43022600	3.16543500	-0.68765400
N	0.61254600	-1.35661600	-0.23932000
C	2.07820200	-1.46947500	-0.41849400
H	2.48148500	-0.47791400	-0.66151500
C	2.59663400	-2.49216900	-1.48205400
O	3.83542900	-2.57289600	-1.51100400
O	1.73323800	-3.08692200	-2.15298300
C	0.00000000	-2.63351000	0.16723100
H	-0.43022600	-3.16543500	-0.68765400
H	0.78780900	-3.29413900	0.55154100
C	-1.05062700	-2.51489900	1.28905900
O	-1.11160900	-1.39318000	1.92756600
O	-1.72792200	-3.49725300	1.53780400

C	0.05794100	0.75966800	-1.42033600
H	-0.35542900	1.19129800	-2.34149700
H	1.11811700	1.04459600	-1.37223100
C	-0.05794100	-0.75966800	-1.42033600
H	-1.11811700	-1.04459600	-1.37223100
H	0.35542900	-1.19129800	-2.34149700
C	1.05062700	2.51489900	1.28905900
O	1.72792200	3.49725300	1.53780400
O	1.11160900	1.39318000	1.92756600
H	-0.78780900	3.29413900	0.55154100
H	2.51610000	-1.73428000	0.55355100
Zn	0.00000000	0.00000000	1.22730400

Cluster: $[EDTA•V]^{2-}$: iso A (^4A)

N	-1.47343700	0.06502300	0.85840600
C	-2.41915400	1.09990200	0.43427300
H	-1.93286200	2.07838800	0.54072800
H	-3.34966600	1.09266700	1.02834000
C	-2.75783100	0.93314300	-1.07512900
O	-3.85291000	1.35537200	-1.44994200
O	-1.84797700	0.39050300	-1.76753300
C	-2.10498600	-1.25663200	0.94429200
H	-2.43393300	-1.48094300	1.97353900

N	1.47328000	-0.06532600	0.85840400
C	2.41899000	-1.10012800	0.43404000
H	1.93264900	-2.07862100	0.54018800
H	3.34946100	-1.09309500	1.02817600
C	2.75773200	-0.93300100	-1.07531100
O	3.85302700	-1.35469300	-1.45009800
O	1.84803600	-0.38989600	-1.76754500
C	2.10492200	1.25626000	0.94469500
H	2.43391300	1.48026500	1.97399000
H	3.00353200	1.24260900	0.31293400
C	1.23809200	2.41723900	0.40510200
O	0.35764000	2.07709300	-0.43518500
O	1.50094500	3.54879400	0.81865800
C	-0.66013300	0.38997500	2.03039000
H	-0.45102600	1.46729800	2.01026900
H	-1.20211200	0.17652300	2.97368900
C	0.65992000	-0.39057600	2.03028200
H	1.20187800	-0.17745100	2.97366600
H	0.45077300	-1.46788900	2.00978800
C	-1.23795400	-2.41738800	0.40459900
O	-1.50050800	-3.54898400	0.81824000
O	-0.35766300	-2.07702600	-0.43575900
H	-3.00361500	-1.24296500	0.31256000

V	-0.00000900	0.00014200	-0.74807000