Electronic supplementary information (ESI)

For

Photoelectron spectroscopic and computational study of [EDTA•*M*(III)]$^-$ complexes (*M* = H_3, Al, Sc, V−Co)

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Table S1 The M-O bond length differences (Å) by subtracting its equatorial bond from its axial bond in the optimized structures of [EDTA•*M*(III)]$^{-}$ (*M* = Al, Sc, V-Co) using five different functionals.

Methods	Al(III)	Sc(III)	V(III)	Cr(III)	Mn(III)	Fe(III)	Co(III) quintet	Co(III) singlet
M06-2X/6-311+G(d,p)	0.055	0.027	0.066	0.019	-0.048	0.056	0.096	0.006
PBE0/6-311+G(d,p)	0.054	0.025	-0.008	0.016	-0.054	0.058	0.098	0.003
B3LYP/6-311+G(d,p)	0.057	0.028	0.067	0.019	-0.045	0.062	0.104	0.004
BHLYP/6-311+G(d,p)	0.054	0.026	0.057	0.017	-0.048	0.055	0.097	0.005
cam-B3LYP/6-311+G(d,p)	0.056	0.028	-0.006	0.019	-0.048	0.062	0.103	0.004

Table S2 Comparison of the experimental ADE/VDE values to the calculated ones (eV) obtained using different functionals for all complexes.

Methods	H	Al(III)	Sc(III)	V(III)	Cr(III)	Mn(III)	Fe(III)	Co(III, quintet)	Co(III, singlet)	Avg. deviation
Expt. VDE	5.35	6.65	6.65	4.4	5.4	5.32	5.72	5.5	5.5	
M06-2X/6-311+G(d,p)	5.32	6.62	6.77	5.37	6.55	6.11	6.54	6.61	6.43	
	-0.03	-0.03	0.12	0.97	1.15	0.79	0.82	1.11	0.93	
	-0.56%	-0.45%	1.80%	22.05%	21.30%	14.85%	14.34%	20.18%	16.91%	12.49%
PBE0/6-311+G(d,p)	4.95	5.79	5.93	4.47	5.47	5.12	5.61	5.69	5.41	
	-0.4	-0.86	-0.72	0.07	0.07	-0.2	-0.11	0.19	-0.09	
	-7.48%	-12.93%	-10.83%	1.59%	1.30%	-3.76%	-1.92%	3.45%	-1.64%	4.99%
B3LYP/6-311+G(d,p)	4.93	5.69	5.82	4.43	5.37	5.07	5.5	5.54	5.42	
	-0.42	-0.96	-0.83	0.03	-0.03	-0.25	-0.22	0.04	-0.08	
	-7.85%	-14.44%	-12.48%	0.68%	-0.56%	-4.70%	-3.85%	0.73%	-1.45%	5.19%
BHLYP/6-311+G(d,p)	5.2	6.44	6.49	5.43	6.52	6.08	6.44	6.34	6.3	
	-0.15	-0.21	-0.16	1.03	1.12	0.76	0.72	0.84	0.8	
	-2.80%	-3.16%	-2.41%	23.41%	20.74%	14.29%	12.59%	15.27%	14.55%	12.14%
cam-B3LYP/6-311+G(d,p)	5.3	6.5	6.64	4.83	5.81	5.62	6.17	6.21	6.36	
	-0.05	-0.15	-0.01	0.43	0.41	0.3	0.45	0.71	0.86	
	-0.93%	-2.26%	-0.15%	9.77%	7.59%	5.64%	7.87%	12.91%	15.64%	6.97%

Methods	H	Al(III)	Sc(III)	V(III)	Cr(III)	Mn(III)	Fe(III)	Co(III)	Avg. deviation
Expt. ADE	4.8	6.1	6.25	3.95	4.9	4.85	5.4	4.85	
M06-2X/6-311+G(d,p)	4.8	5.62	5.8	4.64	5.88	5.63	5.67	2.43	
	0	-0.48	-0.45	0.69	0.98	0.78	0.27	-2.42	
	0.00%	-7.87%	-7.20%	17.47%	20.00%	16.08%	5.00%	-49.90%	15.44%
PBE0/6-311+G(d,p)	4.57	5.42	5.34	3.85	4.86	4.4	5.26	5.11	
	-0.23	-0.68	-0.91	-0.1	-0.04	-0.45	-0.14	0.26	
	-4.79%	-11.15%	-14.56%	-2.53%	-0.82%	-9.28%	-2.59%	5.09%	6.35%
B3LYP/6-311+G(d,p)	4.56	5.28	4.79	3.85	4.78	4.38	5.1	5.12	
	-0.24	-0.82	-1.46	-0.1	-0.12	-0.47	-0.3	0.27	
	-5.00%	-13.44%	-23.36%	-2.53%	-2.45%	-9.69%	-5.56%	5.57%	8.45%
BHLYP/6-311+G(d,p)	4.77	4.87	5.02	4.68	5.77	5.41	6.42	5.67	
	-0.03	-1.23	-1.23	0.73	0.87	0.56	1.02	0.82	
	-0.63%	-20.16%	-19.68%	18.48%	17.76%	11.55%	18.89%	16.91%	15.51%
cam-B3LYP/6-311+G(d,p)	4.81	5.55	5.71	4.16	5.14	4.67	5.58	5.54	
	0.01	-0.55	-0.54	0.21	0.24	-0.18	0.18%	0.69	
	0.21%	-9.02%	-8.64%	5.32%	4.90%	-3.71%	3.33%	14.23%	6.17%

Table S3 Comparison of relative energies for the hexadentate [EDTA•*M*(III)]$^{-}$ (*M* = V-Co) complexes of different spin states at the PBE0/6-311+G(d,p) level.

Cluster	Isomer	RE (eV)
[EDTA•V(III)]$^{-}$	Iso A	
	^{3}A	0
	^{1}A	1.63
[EDTA•Cr(III)]$^{-}$	Iso A	
	^{4}A	0
	^{2}A	1.15
[EDTA•Mn(III)]$^{-}$	Iso A	
	^{5}A	0
	^{3}A	0.94
	^{1}A	2.37
[EDTA•Fe(III)]$^{-}$	Iso A	
	^{6}A	0
	^{4}A	0.85
	^{2}A	0.97
[EDTA•Co(III)]$^{-}$	Iso A	
	^{5}A	0.37
	^{3}A	0.76
	^{1}A	0

Table S4 Comparison of relative energies of different isomers for the [EDTA•*M*(III)]$^{-}$ (*M* = Al, Sc, V-Co) complexes.[a]

Cluster		Isomer	RE (eV)	
[EDTA•H$_3$]$^{-}$		Iso I	0.00	^{1}A→^{2}A
		Iso II	0.08	^{1}A→^{2}A
		Iso III	0.21	^{1}A→^{2}A
[EDTA•Al(III)]$^{-}$	hexadentate	Iso A	0.00	^{1}A→^{2}A
	pentadentate	Iso B	1.21	^{1}A→^{2}A
	tetradentate	Iso C	3.39	^{1}A→^{2}A
[EDTA•Sc(III)]$^{-}$	hexadentate	Iso A	0.00	^{1}A→^{2}A
	pentadentate	Iso B	1.64	^{1}A→^{2}A
	tetradentate	Iso C	3.99	^{1}A→^{2}A
[EDTA•V(III)]$^{-}$	hexadentate	Iso A	0.00	^{3}A→^{2}A
		Iso B	1.63	^{1}A→^{2}A
	pentadentate	Iso C	1.03	^{3}A→^{2}A
	tetradentate	Iso D	2.97	^{3}A→^{2}A
[EDTA•Cr(III)]$^{-}$	hexadentate	Iso A	0.00	^{4}A→^{3}A
		Iso B	1.15	^{2}A→^{1}A
	pentadentate	Iso C	1.42	^{4}A→^{5}A
	tetradentate	Iso D	3.17	^{4}A→^{3}A
[EDTA•Mn(III)]$^{-}$	hexadentate	Iso A	0.00	^{5}A→^{4}A
		Iso B	0.94	^{3}A→^{2}A
	pentadentate	Iso C	1.06	^{5}A→^{4}A
	tetradentate	Iso D	2.25	^{5}A→^{4}A
[EDTA•Fe(III)]$^{-}$	hexadentate	Iso A	0.00	^{6}A→^{5}A
		Iso B	0.85	^{4}A→^{3}A
	pentadentate	Iso C	1.02	^{6}A→^{5}A
	tetradentate	Iso D	2.70	^{6}A→^{7}A
[EDTA•Co(III)]$^{-}$	hexadentate	Iso A	0.00	^{1}A→^{2}A
		Iso B	0.37	^{5}A→^{4}A
	pentadentate	Iso C	1.00	^{3}A→^{4}A
	tetradentate	Iso D	1.99	^{3}A→^{2}A

[a] M06-2X/6-311+G(d,p) for [EDTA•H$_3$]$^{-}$ and [EDTA•Al/Sc]$^{-}$; PBE0/6-311+G(d,p) for [EDTA•*M*]$^{-}$ (*M* = V−Co).

Table S5 Laplacian of electron density ($\nabla^2\rho(r_b)$), and energy density (H_{BCP}) at bond critical points of O−H•••O hydrogen bonds and hydrogen bonding distance obtained by using the atoms in molecules (AIM) methodology with the Multiwfn program.

	$\nabla^2\rho(r_b)$/a.u.	H_{BCP}/a.u.	Distance (Å)
$[EDTAH_3]^-$			
Iso A			
O1-H6•••O2	0.1507	-0.0165	1.551
O4-H7•••O2	0.1276	-0.0002	1.77
O5-H8•••O3	0.1527	-0.0157	1.557
Iso B			
O1-H7•••O2	0.1235	-0.0001	1.779
O3-H8•••O4	0.1186	-0.0446	1.399
O6-H9•••O5	0.1482	-0.0073	1.632
Iso C			
O1-H7•••O2	0.1345	-0.003	1.701
O4-H8•••O3	0.1534	-0.021	1.511
O5-H9•••N6	0.1063	-0.0006	1.963
$[EDTAH_3]$			
O1-H6•••O2	0.1353	0.0008	1.762
O5-H7•••O2	0.0617	0.0024	2.125
O4-H8•••O3	0.108	0.0029	1.87

Table S6 Orbital composition analysis of [EDTA•*M*(III)]$^{-}$ (*M* = Al, Sc, V, Cr, Mn, Fe, Co) for HOMOs which contribute to the first peak (X) by NAO method

EDTA•M(III)	Al(III)				Sc(III)			
	^{1}A				^{1}A			
	HOMO-1	HOMO-2	HOMO-3	HOMO-4	HOMO-1	HOMO-2	HOMO-3	HOMO-4
Exp. (VDE/eV)	**6.60**				**6.70**			
metal atoms (%)	**0.20**	**0.50**	**0.10**	**0.10**	**0.80**	**1.90**	**0.80**	**0.40**
N atoms (%)	10.50	5.70	2.70	2.80	8.20	9.80	2.70	2.50
O atoms (%)	69.20	75.90	79.50	81.20	70.90	66.10	77.10	80.60
C atoms (%)	17.60	16.70	16.90	15.30	18.40	19.60	18.50	16.00

EDTA•M(III)	V(III)	Cr(III)			Mn(III)	Fe(III)		Co(III)	Co(III)
	^{3}A	^{4}A			^{5}A	^{6}A		^{1}A	^{5}A
	HOMO-1	HOMO-1	HOMO-7	HOMO-6	HOMO-1	HOMO-1	HOMO-2	HOMO-1	HOMO-1
Exp. (VDE/eV)	**4.40**	**5.40**			**5.30**	**5.70**		**5.50**	
metal atoms (%)	**66.20**	**41.30**	**7.50**	**0.70**	**14.60**	**4.00**	**8.30**	**1.70**	**5.60**
N atoms (%)	4.20	1.30	1.10	1.70	30.60	22.10	9.40	1.50	6.40
O atoms (%)	24.40	53.10	79.30	86.80	42.60	59.20	75.80	83.10	81.70
C atoms (%)	4.30	3.90	11.20	10.30	7.30	10.80	5.00	13.40	5.40

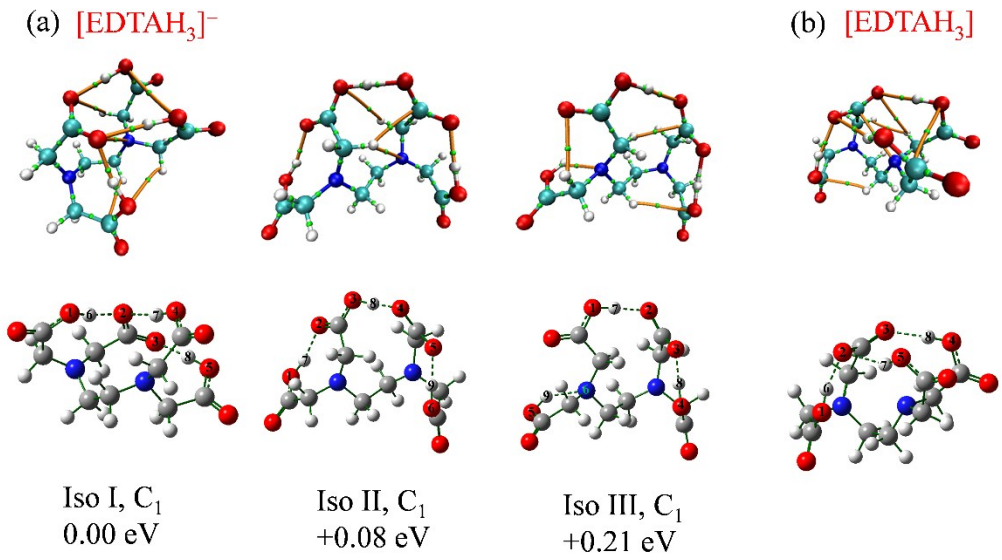

Fig S1 Molecular graph of $[EDTA{\bullet}H_3]^-$ by using the atoms in molecules (AIM) methodology with the Multiwfn program. The green points are bond critical points and the orange lines are bond paths.

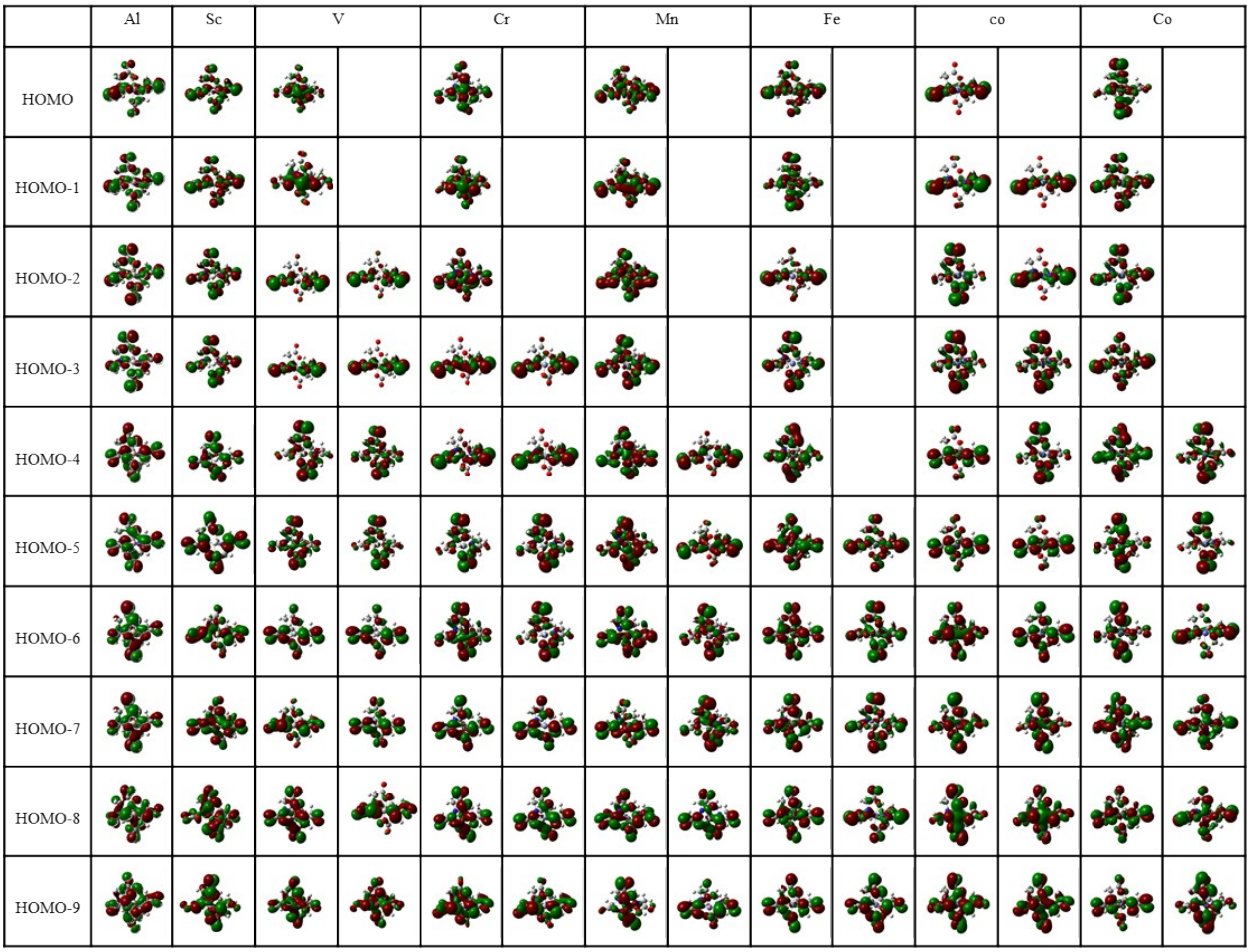

Fig S2 Molecular orbital pictures (HOMO to HOMO-10) of the most stable isomers for [EDTA•*M*(III)]$^{-}$ (*M* = Al, Sc, V, Cr, Mn, Fe, Co)

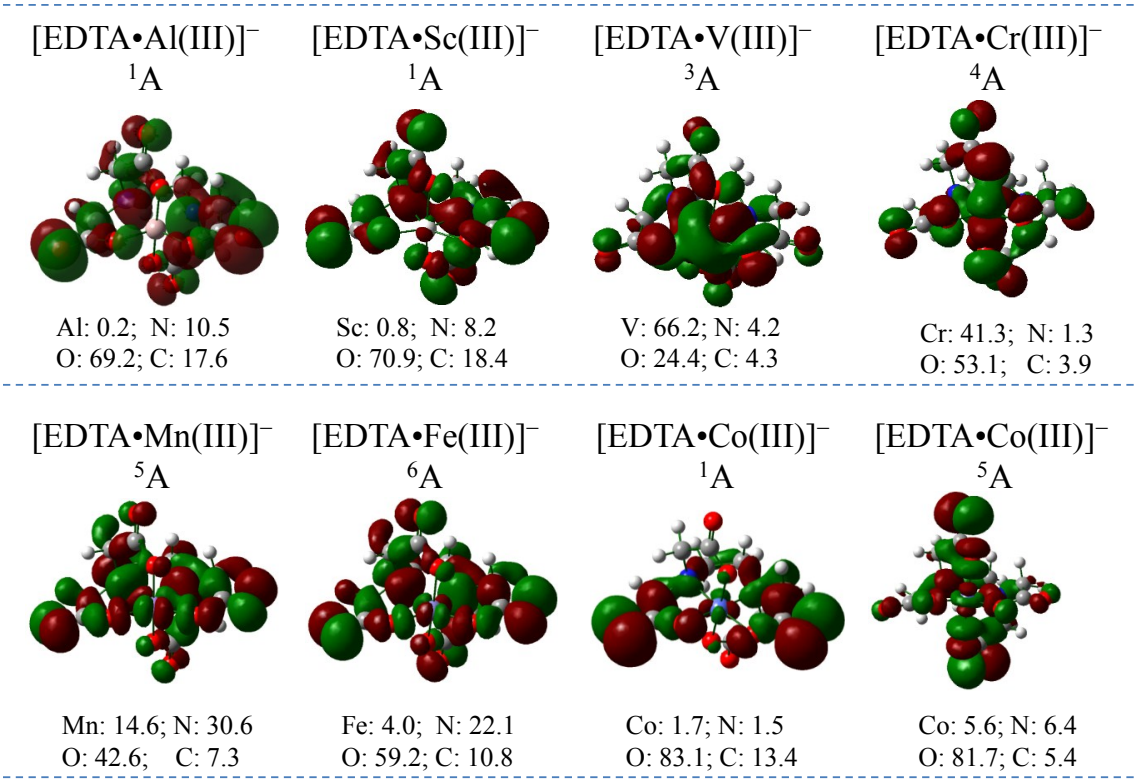

Fig S3 Atom contribution (%) of the *M*, N, O and C in the HOMO pictures of the most stable isomers of [EDTA•*M*(III)]⁻ (*M* = Al, Sc, V, Cr, Mn, Fe, Co).

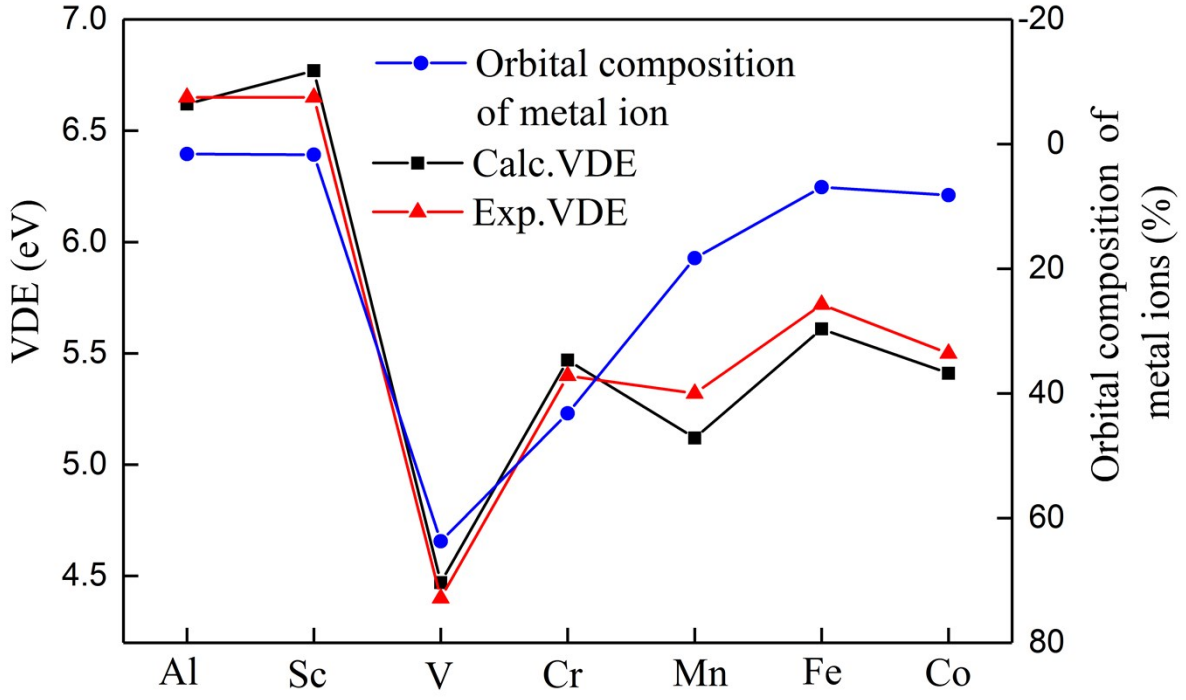

Fig S4 The comparison of the trend of metal atom contribution (%) in HOMOs with the experimental VDEs and ADEs for $[EDTA•M(III)]^-$ (*M* = Al, Sc, V, Cr, Mn, Fe, Co).

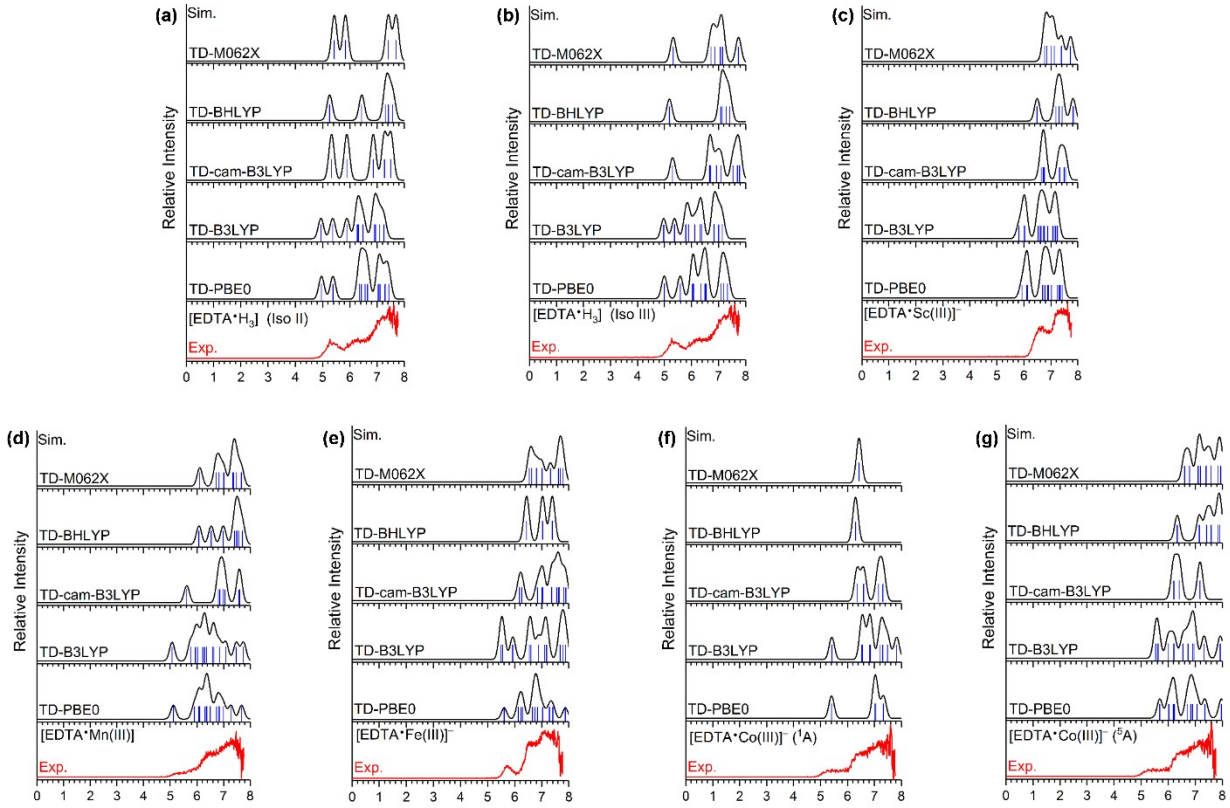

Fig S5 TDDFT simulated spectra of the lowest isomers for [EDTA•M(III)]$^-$ (*M* = H3, Sc, Mn, Fe and Co) using five different functionals, in comparison with the corresponding experimental spectra.

Cartesian coordinates for optimized isomers.

Cluster: $[EDTA•H_3]^-$: iso I (^1A)

N	-2.33015900	-1.11052400	0.42523400
C	-3.29192000	-0.06992200	0.21975700
H	-3.87589200	0.08780100	1.13439700
H	-3.99620200	-0.38227900	-0.55939100
C	-2.80929700	1.33847700	-0.18609300
O	-3.41786600	2.31010900	0.19690000
O	-1.75355900	1.43455500	-0.96418200
C	-1.95038500	-2.03296500	-0.62328700
H	-1.93380200	-3.05816700	-0.23844600
N	0.54818100	0.17098100	0.90375500
C	1.57693000	-0.75773400	1.37780400
H	1.14025700	-1.75679300	1.43760300
H	1.93800200	-0.45681500	2.37354600
C	2.82434900	-0.83345000	0.48541200
O	3.84990900	-0.30072400	0.83143700
O	2.72987900	-1.53318500	-0.62490700
C	1.06254900	1.53237200	0.78933900
H	0.21119300	2.21848000	0.76919400
H	1.71133800	1.81403500	1.63067200
C	1.83552800	1.87431300	-0.48643800

O	1.60310200	1.15586300	-1.56995100
O	2.57447000	2.82391600	-0.49602600
C	-1.53684400	-1.07828200	1.63376800
H	-2.21374500	-1.06997800	2.50223700
H	-0.97063600	-2.01307000	1.68132900
C	-0.60036400	0.12570800	1.81020000
H	-1.18647000	1.03640200	1.66723800
H	-0.26320800	0.13980600	2.86372500
C	-0.56201400	-1.69485800	-1.17721400
O	0.36567400	-2.48314800	-0.90878100
O	-0.46070200	-0.60270300	-1.79858500
H	-2.68535400	-1.96437300	-1.42896000
H	0.91900000	0.45431100	-1.46634700
H	1.80018200	-1.88846900	-0.79572800
H	-1.33925800	0.55648100	-1.26072300

Cluster: $[EDTA•H_3]^-$: iso II (^1A)

N	-1.55131300	-0.26332200	0.96778700
C	-1.77829300	1.16356400	1.08402400
H	-0.86485800	1.65478900	1.42042600
H	-2.55588400	1.38811800	1.82977100
C	-2.25047300	1.77929500	-0.25534200
O	-1.70714200	2.85593400	-0.62786500

O	-3.13183100	1.15894200	-0.87462700
C	-2.69591800	-1.13642400	1.08218900
H	-2.63601900	-1.78296600	1.96733700
N	1.45825800	-0.36831700	-0.42079700
C	0.87875800	0.87879200	-0.84845300
H	-0.20751900	0.81149900	-0.86821100
H	1.17206800	1.13496600	-1.87485400
C	1.36120000	2.05121000	0.02664400
O	0.64610000	3.13666800	0.04383100
O	2.41464100	1.95390500	0.63333000
C	2.60046800	-0.89036200	-1.12293100
H	2.39018700	-1.81861300	-1.66822500
H	2.95406100	-0.15316900	-1.85130700
C	3.79133700	-1.17223100	-0.19657800
O	3.94536700	-0.32264900	0.80786600
O	4.54929300	-2.08756000	-0.38934400
C	-0.26858200	-0.83752400	1.33489800
H	0.33112900	-0.10122200	1.88188600
H	-0.44746000	-1.67787600	2.01849700
C	0.57574700	-1.36892800	0.16176600
H	1.21938800	-2.16911800	0.54190300
H	-0.09780700	-1.81680300	-0.58722800
C	-2.85659400	-2.05560000	-0.13355200

O	-2.99099600	-1.43434500	-1.29343400
O	-2.85525700	-3.25804700	-0.03891800
H	-3.60064900	-0.52514800	1.14536700
H	-0.36445500	3.02670500	-0.27509100
H	3.27387300	0.40148100	0.76718100
H	-3.02198000	-0.44469500	-1.15908300

Cluster: $[EDTA•H_3]^-$: iso III (^1A)

N	-1.87887500	0.35445000	-1.12037800
C	-2.20919600	-1.04454700	-1.28073800
H	-1.58192300	-1.49276500	-2.05612300
H	-3.25031700	-1.14643700	-1.61378500
C	-2.05622800	-1.88292000	0.01579700
O	-1.54740400	-3.01740900	-0.10381900
O	-2.42130000	-1.33566000	1.08260100
C	-2.89900200	1.29379200	-0.74170000
H	-2.97918400	2.11775500	-1.46305000
N	1.39145900	0.26116700	-0.19131400
C	0.74598500	-0.98275200	0.18071800
H	0.06552100	-1.24805300	-0.62218800
H	0.13900700	-0.90544100	1.09685500
C	1.67925800	-2.17756400	0.29634300
O	1.05317900	-3.33142100	0.47951600

O	2.87949100	-2.10311500	0.22478700
C	2.33271100	0.77399500	0.80092900
H	1.87262500	1.46423800	1.51740900
H	2.77769500	-0.05619800	1.35117500
C	3.49691900	1.48949300	0.11881600
O	3.68484000	1.11687600	-1.14828400
O	4.19956000	2.28932600	0.67119200
C	-0.62871500	0.90718100	-1.60007200
H	-0.16440600	0.20573300	-2.30219000
H	-0.85710900	1.81821000	-2.17062100
C	0.40678600	1.30591900	-0.52881600
H	0.97925400	2.16580000	-0.89354200
H	-0.12763300	1.63089900	0.37637500
C	-2.70684300	1.95035000	0.63631400
O	-2.82675200	3.14493700	0.77809000
O	-2.42016900	1.13689800	1.62738900
H	-3.86160500	0.77307000	-0.70668500
H	0.06595500	-3.25570600	0.37823100
H	2.97620900	0.46611400	-1.33219400
H	-2.42377800	0.15232000	1.34485700

Cluster: $[EDTA•Al]^-$: iso A (^1A)

N	1.41462700	0.00945600	0.87207500

C	2.41844600	-0.94947100	0.37894600
H	2.06495200	-1.96685600	0.54905400
H	3.39489500	-0.81234600	0.85102300
C	2.55649000	-0.76057200	-1.15550500
O	3.58207400	-1.10851200	-1.69719900
O	1.52501000	-0.21844700	-1.72508400
C	1.95739000	1.37888800	0.92698700
H	2.23976600	1.66575100	1.94401900
N	-1.41486000	-0.00965000	0.87209000
C	-2.41868300	0.94931800	0.37905200
H	-2.06527000	1.96669200	0.54938000
H	-3.39516900	0.81204000	0.85100300
C	-2.55655900	0.76061900	-1.15544500
O	-3.58193400	1.10900100	-1.69725000
O	-1.52495700	0.21875600	-1.72506800
C	-1.95747400	-1.37914800	0.92665600
H	-2.24002000	-1.66621500	1.94358400
H	-2.85005400	-1.43140900	0.29816700
C	-0.95992800	-2.39284400	0.34846000
O	-0.11347800	-1.86661100	-0.46488200
O	-1.03342700	-3.56091400	0.67656300
C	0.68411900	-0.35156800	2.09657400
H	0.55008500	-1.43567900	2.10976700

H	1.24667400	-0.07189200	2.99550400
C	-0.68438900	0.35113900	2.09667500
H	-1.24694500	0.07121000	2.99552200
H	-0.55038700	1.43524600	2.11016100
C	0.96013600	2.39283300	0.34872000
O	1.03371000	3.56084100	0.67703600
O	0.11366000	1.86678700	-0.46470600
H	2.85011300	1.43113100	0.29870000
Al	0.00003200	0.00010100	-0.72977300

Cluster: $[EDTA•Al]^-$: iso B (^1A)

N	-1.17053100	0.18301500	-0.29608200
C	-1.77281000	-0.87254600	0.59301200
H	-2.30617500	-0.35370400	1.39157300
H	-0.97166600	-1.46414400	1.04345100
C	-2.73892800	-1.81140100	-0.20796300
O	-2.40449500	-3.00804100	-0.22143600
O	-3.67565600	-1.21773300	-0.76853600
C	-2.01630400	1.39929200	-0.32527500
H	-1.78216500	1.97211100	-1.22682400
N	1.29040000	-0.93580600	-0.53990400
C	2.42347200	-0.33005400	-1.26329900
H	2.66139000	-0.86945700	-2.18304200

H	3.30573000	-0.35278300	-0.61549700
C	2.16701500	1.15243200	-1.56853900
O	2.69702100	1.68901100	-2.50837500
O	1.38176200	1.72956100	-0.69716600
C	1.74200900	-1.88611700	0.48742200
H	0.93162600	-2.58118100	0.72172700
H	2.61048700	-2.47072300	0.17494500
C	2.07317500	-1.12084900	1.78004200
O	1.46119400	0.03439600	1.88353100
O	2.80744800	-1.60073300	2.60440400
C	-0.82959700	-0.34785900	-1.63680400
H	-1.71997600	-0.74984600	-2.12602000
H	-0.43532900	0.48289800	-2.22843700
C	0.22402100	-1.43761900	-1.44596500
H	-0.25234200	-2.30965700	-0.99437300
H	0.64324200	-1.73661400	-2.41057700
C	-1.65147500	2.28392100	0.88310800
O	-2.39639900	3.15510700	1.25244500
O	-0.47931800	2.00694900	1.40568100
H	-3.07369700	1.13550800	-0.33362200
Al	0.51491200	0.77567700	0.55844400

Cluster: [EDTA•Al]−: iso C (^{1}A)

N	0.00000000	1.42437000	-0.12433000
C	-1.30894700	2.14911000	-0.26353200
H	-1.59278800	2.52722600	0.72156300
H	-2.07389600	1.43254200	-0.57014200
C	-1.27754000	3.34583600	-1.28826000
O	-2.35028100	3.94840300	-1.33510700
O	-0.19779600	3.50453900	-1.88804300
C	1.09647300	2.33773600	0.31743800
H	1.69729600	2.66483600	-0.52765200
N	0.00000000	-1.42437000	-0.12433000
C	1.30894700	-2.14911000	-0.26353200
H	2.07389600	-1.43254200	-0.57014200
C	1.27754000	-3.34583600	-1.28826000
O	2.35028100	-3.94840300	-1.33510700
O	0.19779600	-3.50453900	-1.88804300
C	-1.09647300	-2.33773600	0.31743800
H	-1.69729600	-2.66483600	-0.52765200
H	-0.65284600	-3.23852200	0.74562900
C	-1.96929200	-1.68901900	1.40381300
O	-1.44489900	-0.58336500	1.95334500
O	-3.00911800	-2.16978400	1.74245300
C	0.35065800	0.67704800	-1.38501300
H	0.07817000	1.29384400	-2.24157400

H	1.43534000	0.54162800	-1.39711300
C	-0.35065800	-0.67704800	-1.38501300
H	-1.43534000	-0.54162800	-1.39711300
H	-0.07817000	-1.29384400	-2.24157400
C	1.96929200	1.68901900	1.40381300
O	3.00911800	2.16978400	1.74245300
O	1.44489900	0.58336500	1.95334500
H	0.65284600	3.23852200	0.74562900
H	1.59278800	-2.52722600	0.72156300
Al	0.00000000	0.00000000	1.17719000

Cluster: $[EDTA•Sc]^-$: iso A (^1A)

N	-1.44768600	-0.08820300	0.85949400
C	-2.53498400	0.83044400	0.47925500
H	-2.18546800	1.85795900	0.60349900
H	-3.43864200	0.67869800	1.07900300
C	-2.87602000	0.66174600	-1.02164000
O	-3.98817900	0.94630600	-1.40868700
O	-1.88693500	0.23455000	-1.74633300
C	-1.92600000	-1.48017700	0.94168800
H	-2.23947100	-1.74269300	1.95775900
N	1.44771900	0.08833900	0.85942600
C	2.53501000	-0.83036300	0.47930100

H	2.18551700	-1.85786300	0.60373700
H	3.43869000	-0.67849800	1.07898500
C	2.87598400	-0.66190500	-1.02163200
O	3.98811300	-0.94657000	-1.40868800
O	1.88686400	-0.23484300	-1.74635500
C	1.92602100	1.48033200	0.94134300
H	2.23960600	1.74301800	1.95733300
H	2.79214800	1.58695400	0.28157800
C	0.88102700	2.48933400	0.43365200
O	0.09226900	2.00404000	-0.46550900
O	0.87730500	3.62142600	0.87482400
C	-0.69937600	0.31316400	2.06241300
H	-0.62181000	1.40270500	2.06880700
H	-1.23270500	0.01469300	2.97544700
C	0.69946400	-0.31281000	2.06244900
H	1.23282700	-0.01416100	2.97540600
H	0.62191000	-1.40234900	2.06905600
C	-0.88114800	-2.48931500	0.43396900
O	-0.87709600	-3.62119200	0.87569000
O	-0.09233800	-2.00414000	-0.46521000
H	-2.79220700	-1.58688000	0.28204600
Sc	-0.00002500	-0.00008800	-0.98989200

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

N	1.28542400	0.06287800	0.39332400
C	1.58049800	-1.11858300	-0.46620100
H	2.25641000	-0.79417600	-1.26008400
H	0.65278300	-1.48043600	-0.93865300
C	2.23783200	-2.31961300	0.31484500
O	1.68379200	-3.41517500	0.14044400
O	3.20375300	-1.98382400	1.01806400
C	2.40367800	1.02208500	0.40335500
H	2.24490100	1.73825300	1.21521400
N	-1.40252100	-0.66476300	0.62377600
C	-2.41843700	0.18178700	1.28258000
H	-2.76012400	-0.25582700	2.22504300
H	-3.28240600	0.26600600	0.61416800
C	-1.92900300	1.62025700	1.51461900
O	-2.28445200	2.24654900	2.48242200
O	-1.16261700	2.06199600	0.55002300
C	-2.04174000	-1.68502200	-0.22907500
H	-1.31079600	-2.46963700	-0.44893000
H	-2.90657500	-2.15176200	0.25184500
C	-2.46937600	-1.07176900	-1.57746100
O	-1.71149000	-0.07375400	-1.95967700
O	-3.40147900	-1.52929500	-2.19056300

C	0.78866400	-0.29996600	1.73826400
H	1.57155100	-0.80780900	2.30926000
H	0.51495400	0.63083400	2.24457900
C	-0.42063700	-1.22236400	1.59139000
H	-0.08439400	-2.19305900	1.22390100
H	-0.88826000	-1.37780900	2.56926400
C	2.41399100	1.83158900	-0.90869200
O	3.38859400	2.45980700	-1.23512900
O	1.27519500	1.78508500	-1.56740800
H	3.35652200	0.51286100	0.56216900
Sc	-0.34990800	0.88353500	-0.83688700

Cluster: $[EDTA•Sc]^-$: iso C (^1A)

N	0.00000000	1.34778100	-0.43245600
C	-1.43733400	1.48831700	-0.12943900
H	-1.55231900	2.06791800	0.79651200
H	-1.90803800	0.49418900	-0.00325000
C	-2.35416600	2.25124600	-1.22674600
O	-3.54898400	2.02810900	-1.06512700
O	-1.69619000	2.93598500	-2.01400200
C	0.75207500	2.58636300	-0.16485700
H	1.70277000	2.54245900	-0.70162000
N	0.00000000	-1.34778100	-0.43245600

C	1.43733400	-1.48831700	-0.12943900
H	1.90803800	-0.49418900	-0.00325000
C	2.35416600	-2.25124600	-1.22674600
O	3.54898400	-2.02810900	-1.06512700
O	1.69619000	-2.93598500	-2.01400200
C	-0.75207500	-2.58636300	-0.16485700
H	-1.70277000	-2.54245900	-0.70162000
H	-0.20631800	-3.46312100	-0.51991100
C	-1.08769100	-2.71976400	1.33338000
O	-0.84950400	-1.62377200	2.04007500
O	-1.54192000	-3.74020100	1.77319500
C	0.27982600	0.70923900	-1.74076800
H	-0.15300700	1.30036000	-2.55029000
H	1.36581600	0.68326700	-1.85824300
C	-0.27982600	-0.70923900	-1.74076800
H	-1.36581600	-0.68326700	-1.85824300
H	0.15300700	-1.30036000	-2.55029000
C	1.08769100	2.71976400	1.33338000
O	1.54192000	3.74020100	1.77319500
O	0.84950400	1.62377200	2.04007500
H	0.20631800	3.46312100	-0.51991100
H	1.55231900	-2.06791800	0.79651200
Sc	0.00000000	0.00000000	1.29156700

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

N	-1.47509000	0.02029300	0.87667600
C	-2.45034400	1.02191600	0.41994700
H	-2.03514600	2.01986500	0.57521400
H	-3.40980600	0.94155900	0.94268300
C	-2.67121600	0.86353400	-1.10474200
O	-3.72044000	1.24474800	-1.58608100
O	-1.67616700	0.33608000	-1.74452600
C	-2.07778300	-1.31593900	0.95161800
H	-2.42013300	-1.55397500	1.96576200
N	1.47514700	-0.02017000	0.87657100
C	2.45042100	-1.02184000	0.41997500
H	2.03533200	-2.01977400	0.57560700
H	3.40995400	-0.94124900	0.94255100
C	2.67101700	-0.86402400	-1.10481500
O	3.72058500	-1.24444500	-1.58603100
O	1.67600400	-0.33648100	-1.74458400
C	2.07781600	1.31608700	0.95123700
H	2.42020900	1.55431500	1.96532100
H	2.95151300	1.34332000	0.29347900
C	1.12676800	2.39469800	0.43905900
O	0.17911900	1.92009900	-0.30183100

O	1.30539800	3.56165500	0.72744400
C	-0.68344400	0.35251800	2.07557000
H	-0.54784100	1.43536300	2.09783300
H	-1.22311400	0.07105000	2.99206300
C	0.68359700	-0.35218700	2.07558400
H	1.22333500	-0.07054800	2.99198500
H	0.54800300	-1.43502900	2.09805400
C	-1.12676800	-2.39465600	0.43959600
O	-1.30541800	-3.56156200	0.72817300
O	-0.17916900	-1.92020800	-0.30145600
H	-2.95151000	-1.34327500	0.29390300
V	-0.00003800	-0.00009600	-0.73540100

Cluster: $[EDTA•V]^-$: iso B (^3A)

N	1.19405700	0.16282100	0.35619400
C	1.79950300	-1.00245400	-0.34936600
H	2.24861000	-0.62775100	-1.27412400
H	1.01151700	-1.70339300	-0.64098800
C	2.89995700	-1.80221300	0.44461100
O	3.03922900	-2.96038400	0.03452500
O	3.47387200	-1.17032500	1.35199000
C	2.08336500	1.34625700	0.27876500
H	1.80604800	2.04542000	1.07429700

N	-1.38464100	-0.83604200	0.69690600
C	-2.48063600	-0.08258300	1.32703000
H	-2.73178400	-0.47771300	2.31711800
H	-3.37167700	-0.17208100	0.69589700
C	-2.18201800	1.41418300	1.41679400
O	-2.68815200	2.09914000	2.27507500
O	-1.40124700	1.84080900	0.46099900
C	-1.89135400	-1.95714800	-0.10851900
H	-1.11238800	-2.72101800	-0.19457600
H	-2.77254200	-2.43275000	0.33368700
C	-2.20210200	-1.49954500	-1.53663600
O	-1.50045300	-0.45538600	-1.90465900
O	-2.98752500	-2.09891800	-2.22948100
C	0.76140000	-0.15979700	1.73377000
H	1.61941600	-0.51937000	2.31088600
H	0.38193700	0.76378100	2.18005500
C	-0.32545700	-1.21638900	1.66796600
H	0.11286300	-2.16270500	1.34570700
H	-0.75433900	-1.37935000	2.66378900
C	1.87954400	2.08010600	-1.05102700
O	2.72282900	2.83090000	-1.47998600
O	0.71498600	1.84872600	-1.61509100
H	3.12190900	1.04789300	0.43286000

V	-0.48987000	0.64576400	-0.72624400

Cluster: $[EDTA•V]^-$: iso C (^3A)

N	-1.29885900	0.35456400	-0.42500300
C	-1.92070300	-0.95245600	-0.15119000
H	-2.41334400	-0.90612600	0.82990800
H	-1.15322300	-1.73984600	-0.13518700
C	-3.05676800	-1.46360600	-1.18275700
O	-3.40758200	-2.61442900	-0.94516700
O	-3.38166800	-0.61446100	-2.02090400
C	-2.21534100	1.47412200	-0.14025300
H	-1.94932700	2.32515800	-0.77254400
N	1.29829500	-0.35424200	-0.42422000
C	1.92077700	0.95303600	-0.15247600
H	1.15373700	1.74075400	-0.13875400
C	3.05795400	1.46113700	-1.18386400
O	3.41056700	2.61167600	-0.94729500
O	3.38190200	0.61092200	-2.02139900
C	2.21483900	-1.47353000	-0.13826900
H	1.94858700	-2.32534400	-0.76944000
H	3.24473100	-1.20472500	-0.38138500
C	2.06839600	-1.92252900	1.31438600
O	0.99200600	-1.42003000	1.89872800

O	2.84191400	-2.68509300	1.83023100
C	-0.60686200	0.45182800	-1.73070900
H	-1.30292500	0.19472400	-2.53428400
H	-0.30213600	1.49436300	-1.85221600
C	0.60661700	-0.45313000	-1.73002700
H	0.30194000	-1.49580600	-1.85044700
H	1.30289400	-0.19698500	-2.53372500
C	-2.06851600	1.92483600	1.31194500
O	-2.84144400	2.68869600	1.82672500
O	-0.99269900	1.42197200	1.89719900
H	-3.24532900	1.20501700	-0.38264300
H	2.41209800	0.90838100	0.82937900
V	-0.00087300	0.00025700	1.13870600

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

N	1.43109100	-0.05130700	0.88486100
C	2.39634000	-1.06462200	0.42311000
H	1.96664800	-2.05811500	0.56875100
H	3.35329300	-0.99481500	0.95073500
C	2.60801700	-0.88262900	-1.09731200
O	3.64177400	-1.27700100	-1.60033200
O	1.61966300	-0.31146100	-1.70473000
C	2.05218400	1.28707700	0.94778000

H	2.36981300	1.52931900	1.96767300
N	-1.43092900	0.05152100	0.88511200
C	-2.39630000	1.06470800	0.42332700
H	-1.96664500	2.05824400	0.56877000
H	-3.35318000	0.99492400	0.95109000
C	-2.60814500	0.88256300	-1.09705500
O	-3.64223500	1.27630500	-1.59988600
O	-1.61995900	0.31113500	-1.70450300
C	-2.05199000	-1.28685800	0.94846000
H	-2.36938000	-1.52888500	1.96847800
H	-2.94280700	-1.28416700	0.31442400
C	-1.13776600	-2.38294800	0.39506900
O	-0.24298100	-1.94616700	-0.42128900
O	-1.31770900	-3.53962700	0.73164200
C	0.66685600	-0.37519700	2.10330100
H	0.49364600	-1.45379900	2.11387600
H	1.23783900	-0.12062500	3.00698900
C	-0.66646900	0.37569700	2.10333700
H	-1.23728500	0.12133100	3.00719000
H	-0.49325900	1.45430100	2.11363400
C	1.13781300	2.38304700	0.39439500
O	1.31797200	3.53982600	0.73050700
O	0.24291100	1.94610200	-0.42174800

H	2.94285200	1.28424700	0.31353400
Cr	-0.00005800	-0.00005800	-0.64911400

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

N	1.29070700	0.10730300	0.34288100
C	1.76319700	-0.95229800	-0.58611900
H	2.33694600	-0.47363700	-1.38152700
H	0.89103500	-1.44618100	-1.05145100
C	2.64417900	-2.04949000	0.12437100
O	2.23177100	-3.21235200	-0.00291100
O	3.61271300	-1.57493100	0.73922300
C	2.15762700	1.29458500	0.33094800
H	1.88265300	1.93835700	1.17139300
N	-1.30122700	-0.84696000	0.63259700
C	-2.26722600	-0.06751900	1.43285700
H	-2.47954200	-0.55523800	2.38930500
H	-3.20532000	0.00160700	0.87285700
C	-1.79890800	1.36875500	1.65394100
O	-2.20155000	2.01767000	2.59259100
O	-0.98736700	1.79586000	0.72792600
C	-1.99413400	-1.79071100	-0.26171100
H	-1.27614400	-2.53771500	-0.61585100
H	-2.80844600	-2.32010400	0.24278600

C	-2.53191000	-1.04059100	-1.49829700
O	-1.89594300	0.06357000	-1.76871200
O	-3.44352700	-1.51776300	-2.13581000
C	0.91015900	-0.42560800	1.66687900
H	1.77139900	-0.90805800	2.14068300
H	0.58911800	0.41956800	2.28031600
C	-0.21659400	-1.43486400	1.46580800
H	0.18063900	-2.31432000	0.95205500
H	-0.61159400	-1.76300400	2.43397000
C	1.89074600	2.08306600	-0.96286100
O	2.67886800	2.91168900	-1.35248500
O	0.75940500	1.77579200	-1.55325500
H	3.20839800	1.00934600	0.41920900
Cr	-0.40763600	0.58911500	-0.61873100

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

N	1.41229500	-0.18614000	-0.19752100
C	2.17155400	1.09390500	-0.24206500
H	2.62131300	1.25518100	0.74253100
H	1.47973000	1.91918100	-0.42526100
C	3.32595000	1.15828600	-1.32607300
O	3.96709500	2.20685500	-1.24459900
O	3.41173400	0.17382300	-2.08029400

C	2.30261500	-1.33291700	0.12312600
H	2.52728200	-1.90986300	-0.77328500
N	-1.41314400	0.18493500	-0.19670800
C	-2.16953900	-1.09692800	-0.23891300
H	-1.47580700	-1.92109700	-0.41971600
C	-3.32321300	-1.16649000	-1.32314100
O	-3.96222600	-2.21619400	-1.23919000
O	-3.41091400	-0.18428100	-2.08014600
C	-2.30633300	1.33026800	0.12107200
H	-2.53676400	1.90117400	-0.77775200
H	-3.26324900	0.94709800	0.48254900
C	-1.70977500	2.20231600	1.21572000
O	-0.65373800	1.65171300	1.80625700
O	-2.18520000	3.25927300	1.52993300
C	0.62073300	-0.42900700	-1.44253700
H	1.27116600	-0.22747700	-2.29879800
H	0.35499700	-1.48925000	-1.45697800
C	-0.62225000	0.42776300	-1.44221000
H	-0.35668900	1.48810300	-1.45676800
H	-1.27324200	0.22584700	-2.29799300
C	1.70715600	-2.19693500	1.22480100
O	2.18052200	-3.25346200	1.54349300
O	0.65469300	-1.63988600	1.81563500

H	3.26243300	-0.95139000	0.47849100
H	-2.61920400	-1.25695000	0.74589100
Cr	0.00070300	0.00431600	1.24122100

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

N	-1.43846400	-0.02882600	0.98750600
C	-2.46478300	0.92389700	0.57481600
H	-2.08731700	1.93965400	0.72289300
H	-3.40220500	0.81117700	1.13411200
C	-2.75312900	0.77833000	-0.92989400
O	-3.83279600	1.13360300	-1.36390100
O	-1.77931600	0.27918400	-1.61351300
C	-1.92724700	-1.40901100	1.00040400
H	-2.09387000	-1.77372100	2.02144600
N	1.43844300	0.02906200	0.98736200
C	2.46470200	-0.92377400	0.57476700
H	2.08716900	-1.93949200	0.72295100
H	3.40212400	-0.81106300	1.13406200
C	2.75311900	-0.77834400	-0.92995100
O	3.83256500	-1.13424600	-1.36399500
O	1.77922900	-0.27950200	-1.61367600
C	1.92732600	1.40921700	1.00004000
H	2.09376500	1.77416300	2.02103100

H	2.89186900	1.44915600	0.48449500
C	1.02167200	2.39922400	0.26324800
O	0.20776400	1.88042400	-0.60510900
O	1.11540700	3.58638400	0.50432100
C	-0.68622000	0.33387600	2.18173200
H	-0.56964900	1.42161500	2.19021000
H	-1.22483100	0.05726800	3.10257500
C	0.68627600	-0.33343100	2.18170900
H	1.22496900	-0.05670100	3.10246800
H	0.56968300	-1.42116600	2.19035600
C	-1.02123300	-2.39909200	0.26416200
O	-1.11564300	-3.58630200	0.50473100
O	-0.20762600	-1.88047700	-0.60458600
H	-2.89167500	-1.44917200	0.48465300
Mn	0.00002200	-0.00005100	-0.83902800

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

N	1.22672700	0.14100500	0.33052700
C	1.92306000	-0.97317200	-0.37145400
H	2.26661900	-0.59128600	-1.33583700
H	1.21280200	-1.77715000	-0.58478200
C	3.16057100	-1.60422300	0.38050400
O	3.49361800	-2.68779700	-0.10880700

O	3.62242800	-0.93978500	1.32596600
C	1.98886800	1.40148300	0.20928200
H	1.61744100	2.10914500	0.95645600
N	-1.32311600	-0.88011800	0.68143800
C	-2.39932800	-0.12739900	1.36931100
H	-2.64309600	-0.59707200	2.32683900
H	-3.29242500	-0.15787500	0.73730000
C	-2.05760800	1.36067100	1.56209400
O	-2.57603100	1.96424400	2.48138000
O	-1.25901900	1.82120800	0.66553300
C	-1.88825300	-1.96438300	-0.14268500
H	-1.09427100	-2.67230100	-0.40116200
H	-2.67520400	-2.51321000	0.38292500
C	-2.42771200	-1.38367900	-1.46316500
O	-1.85664000	-0.26693900	-1.81561700
O	-3.27704100	-1.97912700	-2.08415000
C	0.82360500	-0.21961900	1.71172900
H	1.70637500	-0.56593700	2.25851000
H	0.42793900	0.68181600	2.18320300
C	-0.24173100	-1.29685900	1.62253900
H	0.19530000	-2.22493100	1.24960900
H	-0.66262800	-1.50594500	2.61156100
C	1.70980600	2.00952200	-1.16736300

O	2.43199000	2.83912100	-1.65739400
O	0.60227900	1.55976800	-1.73195500
H	3.05177600	1.22328600	0.38077300
Mn	-0.49744900	0.48262600	-0.66854200

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

N	1.33085400	0.38828100	-0.29867700
C	2.06601600	0.31364800	0.99492000
H	2.56141800	-0.66036900	1.04904800
H	1.35691400	0.38285000	1.82675900
C	3.18238200	1.42942700	1.23590900
O	3.64017800	1.36272000	2.37492500
O	3.41685600	2.16488400	0.26475700
C	2.20502500	0.00497700	-1.42760300
H	1.79371200	0.41840500	-2.35328900
N	-1.33084800	0.38830800	0.29850000
C	-2.06604600	0.31338900	-0.99503700
H	-1.35701400	0.38260400	-1.82694000
C	-3.18250700	1.42906900	-1.23597600
O	-3.64027600	1.36236800	-2.37500200
O	-3.41675900	2.16466400	-0.26487900
C	-2.20501200	0.00525200	1.42750000
H	-1.79369700	0.41888600	2.35309400

H	-3.20367100	0.42362200	1.28907100
C	-2.22497800	-1.51845600	1.57333600
O	-1.24336300	-2.13240200	0.92813900
O	-3.04510100	-2.07715300	2.25096800
C	0.59767100	1.67673500	-0.46359200
H	1.28869900	2.49962000	-0.26066400
H	0.27984400	1.74333900	-1.50656400
C	-0.59773300	1.67682800	0.46310600
H	-0.27990800	1.74369800	1.50606200
H	-1.28881600	2.49962000	0.25995600
C	2.22498200	-1.51875900	-1.57313300
O	3.04520300	-2.07761600	-2.25051500
O	1.24341000	-2.13258900	-0.92775800
H	3.20367500	0.42339600	-1.28926800
H	-2.56138000	-0.66066800	-1.04901900
Mn	0.00000800	-1.08011200	0.00005300

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

N	1.44224500	0.02543400	0.92019800
C	2.45115200	-0.94403500	0.48140900
H	2.06076300	-1.95388700	0.62935200
H	3.39754500	-0.84009100	1.02468600
C	2.70383200	-0.79424900	-1.03095700

O	3.76554200	-1.15387900	-1.49689700
O	1.70913500	-0.28929600	-1.69359000
C	1.98057100	1.38838500	0.97921400
H	2.27175200	1.66465100	1.99961600
N	-1.44231500	-0.02520900	0.92011700
C	-2.45116700	0.94417200	0.48101700
H	-2.06074500	1.95405300	0.62867400
H	-3.39758400	0.84042400	1.02428900
C	-2.70381200	0.79390800	-1.03130500
O	-3.76536300	1.15374800	-1.49744500
O	-1.70905200	0.28885500	-1.69376300
C	-1.98063200	-1.38815400	0.97938300
H	-2.27202200	-1.66415000	1.99979700
H	-2.87870600	-1.43771000	0.35650400
C	-1.01647700	-2.43479400	0.41238500
O	-0.15425500	-1.95955200	-0.41704000
O	-1.13528700	-3.59930300	0.75075800
C	0.68510600	-0.33853400	2.11967500
H	0.56666000	-1.42468800	2.12983400
H	1.22917400	-0.05825000	3.03437300
C	-0.68525300	0.33902600	2.11955900
H	-1.22937600	0.05894600	3.03428600
H	-0.56680400	1.42518200	2.12948800

C	1.01661200	2.43490700	0.41167500
O	1.13509400	3.59942600	0.75012800
O	0.15430500	1.95942500	-0.41752600
H	2.87878200	1.43775000	0.35651900
Fe	0.00001900	-0.00011500	-0.80919100

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

N	1.22195600	0.15836800	0.38111800
C	1.83667500	-0.96878800	-0.36621300
H	2.24583200	-0.56243300	-1.29545900
H	1.06289300	-1.68657400	-0.65149400
C	2.98363800	-1.75458300	0.37810200
O	3.17072500	-2.88186300	-0.09349600
O	3.53870400	-1.14398600	1.31128500
C	2.07713900	1.35760900	0.33628300
H	1.79318700	2.02756100	1.15435900
N	-1.32079300	-0.93291200	0.70581600
C	-2.44353300	-0.23603100	1.35025300
H	-2.66046000	-0.64939200	2.34112600
H	-3.33877300	-0.37257000	0.73381700
C	-2.24875900	1.27850500	1.45990500
O	-2.82515600	1.90470400	2.31939100
O	-1.47861800	1.78769900	0.53843500

C	-1.78329500	-2.01228300	-0.17224300
H	-0.96690700	-2.72316600	-0.33296100
H	-2.62608900	-2.56911400	0.25104800
C	-2.16868500	-1.47578300	-1.55747300
O	-1.56855300	-0.36339600	-1.88467100
O	-2.93492200	-2.09421800	-2.25844400
C	0.79958100	-0.21555100	1.74452100
H	1.66991600	-0.56076200	2.31211100
H	0.38676800	0.68114600	2.21662100
C	-0.25130600	-1.30809100	1.65496300
H	0.21408000	-2.23260000	1.30822300
H	-0.66687000	-1.50790100	2.65000700
C	1.84752700	2.12604200	-0.96733000
O	2.63595800	2.95451000	-1.35213700
O	0.71983900	1.82145300	-1.57147400
H	3.12592100	1.08442200	0.46971100
Fe	-0.51943700	0.68721900	-0.69236000

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

N	1.33064700	0.33429600	0.45953600
C	1.95345100	-0.96735500	0.23131900
H	2.45137800	-0.97260800	-0.74351300
H	1.20970600	-1.77112200	0.26699500

C	3.11641600	-1.42517100	1.29523000
O	3.48256300	-2.57186100	1.07329000
O	3.41212900	-0.54704000	2.10730200
C	2.21212900	1.46006500	0.12465900
H	1.90523100	2.33685700	0.70070000
N	-1.33064900	-0.33428900	0.45950600
C	-1.95347500	0.96736000	0.23134000
H	-1.20973600	1.77113300	0.26707200
C	-3.11645900	1.42507000	1.29525000
O	-3.48255200	2.57180600	1.07345600
O	-3.41218800	0.54685800	2.10723000
C	-2.21211900	-1.46005300	0.12458200
H	-1.90521600	-2.33686000	0.70059800
H	-3.24660200	-1.24368000	0.40141400
C	-2.11422500	-1.84038800	-1.35802900
O	-1.13349900	-1.26298000	-2.01031200
O	-2.89008500	-2.63558100	-1.82973400
C	0.61337500	0.44903500	1.73923800
H	1.28173100	0.19306400	2.56707000
H	0.31778900	1.49488900	1.85351200
C	-0.61339900	-0.44906400	1.73921600
H	-0.31781400	-1.49492100	1.85347400
H	-1.28177400	-0.19311600	2.56704000

C	2.11425400	1.84044900	-1.35794200
O	2.89010500	2.63567800	-1.82960100
O	1.13353200	1.26307300	-2.01025800
H	3.24660800	1.24367400	0.40148900
H	-2.45136300	0.97266300	-0.74351300
Fe	0.00001400	0.00002600	-1.16791500

Cluster: $[EDTA•Co]^-$: iso A (^1A)

N	-1.38209300	0.15441900	0.89741500
C	-2.27087300	1.21569300	0.38755000
H	-1.79974000	2.18714600	0.53842800
H	-3.25153500	1.19206500	0.87207400
C	-2.41036900	0.99074300	-1.13471100
O	-3.38345800	1.43682100	-1.71341400
O	-1.44507100	0.31390700	-1.65760100
C	-2.09895900	-1.14061700	0.94565700
H	-2.41898200	-1.37447800	1.96558300
N	1.38216400	-0.15426400	0.89731500
C	2.27088600	-1.21563800	0.38755200
H	1.79976500	-2.18706200	0.53865000
H	3.25159600	-1.19193100	0.87197600
C	2.41023000	-0.99097200	-1.13477200
O	3.38329600	-1.43711600	-1.71346700

O	1.44491600	-0.31417900	-1.65769000
C	2.09906000	1.14076900	0.94525800
H	2.41916700	1.37481900	1.96511400
H	2.99333000	1.06507700	0.32242500
C	1.26344600	2.27740800	0.36463300
O	0.30695700	1.87470500	-0.39304000
O	1.54504200	3.43285600	0.63048900
C	-0.63405400	0.42646700	2.14025200
H	-0.38057400	1.48858600	2.15435900
H	-1.24510700	0.21249600	3.02618500
C	0.63423700	-0.42608000	2.14027000
H	1.24537100	-0.21195000	3.02610900
H	0.38075800	-1.48819800	2.15459600
C	-1.26334000	-2.27734500	0.36520900
O	-1.54495900	-3.43275500	0.63121000
O	-0.30699800	-1.87476300	-0.39271300
H	-2.99328200	-1.06506700	0.32288000
Co	-0.00002400	-0.00003500	-0.46789100

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

N	1.41219900	0.05654800	0.91646900
C	2.45689100	-0.88097500	0.49431400
H	2.09901800	-1.90319200	0.64233500

H	3.39391600	-0.74052200	1.04519700
C	2.69977100	-0.71751300	-1.01254400
O	3.75479700	-1.05787400	-1.50450300
O	1.68901000	-0.20814100	-1.64627300
C	1.90095500	1.44403200	0.96008800
H	2.17819300	1.73324500	1.98009600
N	-1.41245500	-0.05656500	0.91636900
C	-2.45722600	0.88084500	0.49417400
H	-2.09959400	1.90309500	0.64252700
H	-3.39436300	0.74007500	1.04479000
C	-2.69964000	0.71777000	-1.01279700
O	-3.75491200	1.05731500	-1.50479200
O	-1.68883800	0.20825100	-1.64634700
C	-1.90100100	-1.44411900	0.95985600
H	-2.17846200	-1.73337500	1.97978900
H	-2.79788000	-1.51511600	0.33792700
C	-0.90580500	-2.46355000	0.38267000
O	-0.12869500	-1.99712500	-0.52319000
O	-0.94869300	-3.61316100	0.79407700
C	0.68777500	-0.32532600	2.13042100
H	0.59028800	-1.41389300	2.14213700
H	1.24264400	-0.03178700	3.03354300
C	-0.68815800	0.32531700	2.13038600

H	-1.24309400	0.03173700	3.03345200
H	-0.59069800	1.41388500	2.14213600
C	0.90616800	2.46367300	0.38255200
O	0.94878200	3.61314700	0.79437100
O	0.12893900	1.99730000	-0.52323700
H	2.79801500	1.51486100	0.33840500
Co	0.00008600	0.00009200	-0.76176900

Cluster: $[EDTA•Co]^-$: iso B (^3A)

N	-1.19351100	-0.16486600	0.34253400
C	-1.92859800	0.94689100	-0.31621700
H	-2.23201800	0.59960300	-1.30648500
H	-1.25643200	1.79366200	-0.46935700
C	-3.21398000	1.47441000	0.44129400
O	-3.62033000	2.53498100	-0.04163000
O	-3.62846900	0.77284000	1.38108800
C	-1.90831800	-1.45009900	0.15980300
H	-1.54228200	-2.16268500	0.90437300
N	1.29746300	0.88339500	0.71479500
C	2.42984500	0.16473400	1.33714400
H	2.69374800	0.60986900	2.30082700
H	3.29399300	0.24891900	0.67067800
C	2.13589900	-1.33301300	1.47933900

O	2.67574300	-1.97605400	2.35641100
O	1.33455400	-1.77132600	0.56825700
C	1.77623500	2.02520500	-0.08473700
H	0.95143800	2.72601500	-0.24432800
H	2.58950300	2.56119600	0.41267300
C	2.21512400	1.52643500	-1.46820600
O	1.61375100	0.43183900	-1.83222200
O	3.00828800	2.15774300	-2.12791200
C	-0.81360900	0.13625300	1.74304800
H	-1.70912000	0.43639300	2.29634200
H	-0.40358900	-0.77980500	2.17231800
C	0.23381100	1.22865900	1.70629800
H	-0.21935700	2.17360200	1.40247100
H	0.67624200	1.37858000	2.69626300
C	-1.55731400	-2.01345900	-1.21725000
O	-2.24950000	-2.83586300	-1.76630100
O	-0.43557700	-1.54565800	-1.71771400
H	-2.98087300	-1.30833600	0.29879800
Co	0.50403200	-0.43299300	-0.58440000

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

N	1.43434300	0.19720900	0.22811500
C	2.19098800	-1.04084900	0.27385400

H	2.69786900	-1.19326100	-0.68084400
H	1.53445700	-1.89370600	0.45316900
C	3.35644400	-1.13188700	1.40898200
O	3.97818800	-2.18325600	1.26912800
O	3.41285800	-0.18051900	2.18723600
C	2.26424300	1.36336200	-0.12656200
H	2.51970100	1.94275400	0.76187900
N	-1.43410400	-0.19754100	0.22860400
C	-2.19102200	1.04032100	0.27415700
H	-1.53469700	1.89338700	0.45323200
C	-3.35639100	1.13123700	1.40949700
O	-3.97834000	2.18246800	1.26958600
O	-3.41248700	0.17991200	2.18779500
C	-2.26365900	-1.36398200	-0.12590700
H	-2.51764200	-1.94419200	0.76241800
H	-3.21000100	-1.01270600	-0.54542400
C	-1.61244300	-2.25814400	-1.19194400
O	-0.64692500	-1.69675900	-1.86032400
O	-2.04846200	-3.37166800	-1.37972500
C	0.60872900	0.44438600	1.43497900
H	1.22709100	0.29418400	2.32635800
H	0.31254400	1.49648600	1.41382200
C	-0.60815600	-0.44419400	1.43533300

H	-0.31197600	-1.49629500	1.41458000
H	-1.22625900	-0.29362000	2.32682900
C	1.61230400	2.25861700	-1.19119800
O	2.04852500	3.37213400	-1.37856400
O	0.64592000	1.69808600	-1.85906600
H	3.20982300	1.01168800	-0.54747700
H	-2.69814300	1.19240000	-0.68046600
Co	-0.00018100	0.00032700	-1.32410300