Electronic Supplementary Information (ESI)

Role of EDTA protonation in chelation-based removal of mercury ions from water

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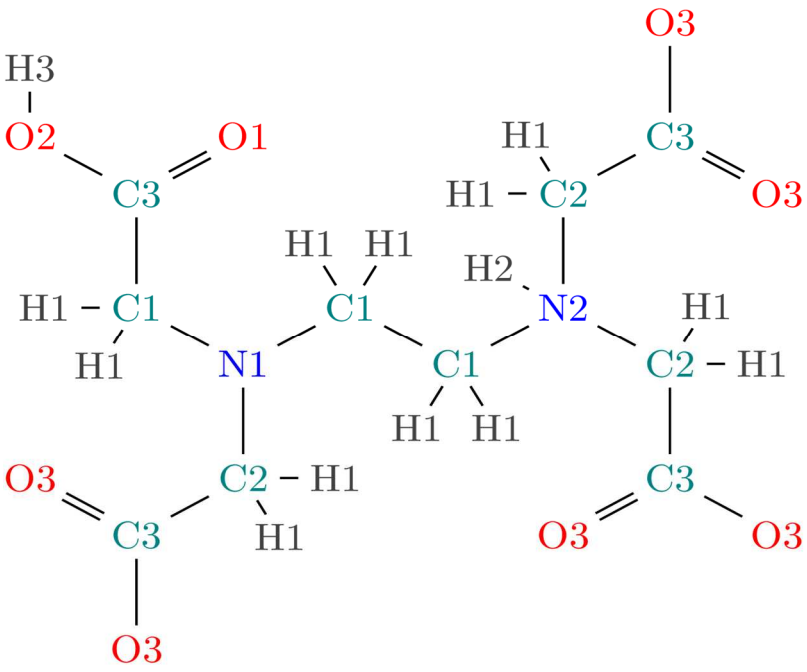


Figure S1. Atomistic model of $EDTA^{2-}$ described using the OPLS/AA force field. The OPLS/AA force field parameters are reported in Tables S1-S5.

Table S1. The non-bonding OPLS/AA parameters for EDTA and the Hg^{2+} ion. Notations for the EDTA atoms correspond to those used in Figure S1. The parameters are used with the Lennard-Jones potential $U_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$ and the Coulomb potential $U_{coul}(r) = \frac{q_i q_j}{\epsilon r}$.

Type	Charge	Mass	ε (kcal mol^{-1})	σ (Å)
N1	-0.63	14.007	0.17	3.3
N2	-0.1	14.007	0.17	3.25
C1	0.09	12.011	0.066	3.5
C2	-0.22	12.011	0.066	3.5
C3	0.7	12.011	0.105	3.75
H1	0.06	1.008	0.03	2.5
H2	0.29	1.008	0.0	0.0
H3	0.45	1.008	0.0	0.0
O1	-0.44	15.999	0.21	2.96
O2	-0.53	15.999	0.17	3.0
O3	-0.8	15.999	0.21	2.96
Hg^{2+}	2	200.59	0.0409	2.36

Table S2. The OPLS/AA parameters for EDTA used for the harmonic bond stretching potential $U_b(r) = K_b(r - r_0)^2$. Notations for the EDTA atoms correspond to those in Figure S1.

Bond	K_b (kcal mol^{-1} Å^{-2})	r_0 (Å)
C1-H1,C2-H1	340.0	1.09
C1-N1,C2-N1	382.0	1.448
C1-C1	268.0	1.529
O2-H3	553.0	0.945
C1-C3	317.0	1.522
C3-O1	570.0	1.229
C3-O2	450.0	1.364
C3-O3	656.0	1.25
N2-C1,N2-C2	367.0	1.471
N2-H2	434.0	1.01

Table S3. The OPLS/AA parameters for EDTA used for the harmonic bond angle potential: $U_a(\theta) = K_a(\theta - \theta_0)^2$. Notations for the EDTA atoms correspond to those used in Figure S1.

Angle	K_a (kcal mol^{-1} rad^{-2})	θ_0 (°)
O2-C3-O1	80.0	121.0
O2-C3-C1	70.0	108.0
O1-C3-C1	80.0	120.4
O3-C3-C2	70.0	117.0
O3-C3-O3	80.0	126.0
C3-O2-H3	35.0	113.0
N1-C1-C1	56.2	109.47
N1-C1-C3,N1-C2-C3	80.0	111.2
H1-C1-H1,H1-C2-H1	33.0	107.8
C3-C1-H1,C3-C2-H1	35.0	109.5
N1-C1-H1,N1-C2-H1	35.0	109.5
C1-C1-H1	37.5	110.7
C1-N1-C1,C1-N1-C2	51.8	107.2
N2-C1-H1,N2-C2-H1	35.0	109.5
N2-C2-C3,N2-C1-C1	80.0	111.2
C1-N2-C2, C2-N2-C2	50.0	113.0
C1-N2-H2,C2-N2-H2	35.0	109.5

Table S4. The OPLS/AA parameters for EDTA used for the dihedral angle potential: $U_{dih}(\phi) = \frac{1}{2}K_1[1 + cos(\phi)] + \frac{1}{2}K_2[1 - cos(2\phi)] + \frac{1}{2}K_3[1 + cos(3\phi)] + \frac{1}{2}K_4[1 - cos(4\phi)]$. Notations for the EDTA atoms correspond to those used in Figure S1.

Dihedral	K_1 (kcal mol^{-1})	K_2 (kcal mol^{-1})	K_3 (kcal mol^{-1})	K_4 (kcal mol^{-1})
O1-C3-O2-H3	0	5.0	0	0
C1-C3-O2-H3	1.5	5.5	0	0
O1-C3-C1-N1	0	0.82	0	0
O1-C3-C1-H1	0	0	0	0
O2-C3-C1-N1	5.26	0.82	0	0
O2-C3-C1-H1	0	0	0	0
O3-C3-C2-N1	0	0.82	0	0
O3-C3-C2-H1	0	0	0	0
N1-C1-C1-N1	11.035	-0.968	0.27	0
N1-C1-C1-H1	-1.013	-0.709	0.473	0
H1-C1-C1-H1	0	0	0.3	0
C1-C1-N1-C1, C1-C1-N1-C2	0.416	-0.128	0.695	0
C1-N1-C1-H1, C2-N1-C1-H1	0	0	0.56	0
N2-C1-C1-H1	0	0	0.384	0
C1-C1-N2-C2	1.438	-0.124	0.264	0
C2-N2-C1-H1, C1-N2-C1-H1	0	0	0.302	0
H1-C1-N2-H2, H1-C2-N2-H2	0	0	0.3	0
C1-N2-C2-C3, C2-N2-C2-C3	1.438	-0.124	0.264	0
C3-C2-N2-H2, C1-C1-N2-H2	0	0	0.347	0

Table S5. The OPLS/AA parameters for EDTA used for the improper dihedral angle potential: $U_{imp}(\chi) = K_{imp}(\chi - \chi_0)^2$. Notations for the EDTA atoms correspond to those used in Figure S1.

Improper	K_{imp} (kcal mol^{-1} rad^{-2})	χ_0 (°)
O3-C2-C3-O3, O3-O3-C3-C2, O1-O2-C3-C1, O2-C1-C3-O1	10.5	180.0

Table S6. Root-mean-square deviation of the $EDTA^{4-}$-Hg^{2+}-water complex in water solvent optimized at various computational levels relative to the experimentally resolved structure using X-ray absorption spectroscopy [1].[a]

Functional	Basis set	Solvent model	RMSD (Å)
B3LYP	Def2-TZVPP	SMD	1.069
HSE06	Def2-TZVPP	SMD	1.257
M05-2X	Def2-TZVPP	SMD	0.941
PBE	Def2-TZVPP	SMD	1.285
PBE0	Def2-TZVPP	SMD	1.089
ωB97X-D	Def2-TZVPP	SMD	1.350
M05-2X	Def2-TZVP	SMD	1.107
M05-2X	LanL2DZ	SMD	0.694
M05-2X	LanL2DZ	CPCM	0.769
M05-2X	LanL2DZ	PCM	0.769
UM05-2X	LanL2DZ	SMD	0.700
UωB97X-D	Def2-TZVPP	SMD	1.141

[a] The starting and optimized structures are shown in Figure S2.

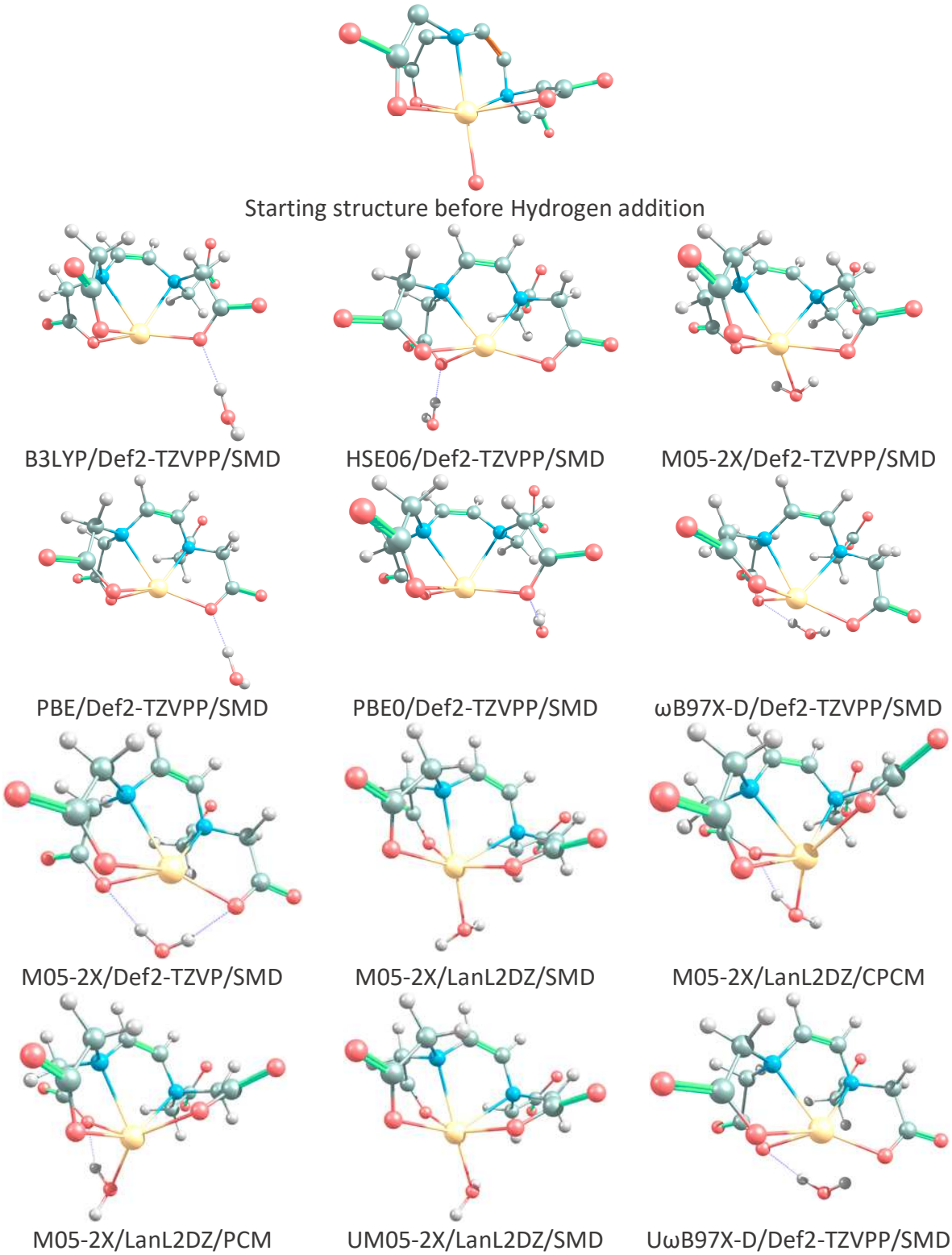


Figure S2. The starting and optimized structures of the $EDTA^{4-}$-Hg^{2+}-water complex in implicit water solvent. The backbone of the starting structure is adopted from Ref. [1] and the missing hydrogens are added to it. The grey, red, blue, white, and yellow balls represent the carbon, oxygen, nitrogen, hydrogen, and mercury atoms, respectively.

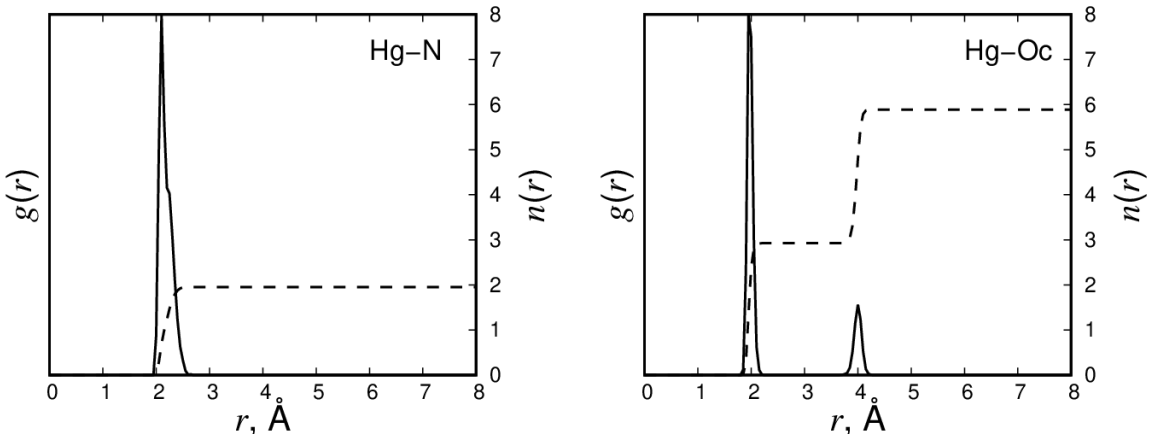


Figure S3. The radial distribution functions *g(r)* (solid line) and running coordination functions *n(r)* (dashed line) for *th*EDTA^{3-}+Hg^{2+}.

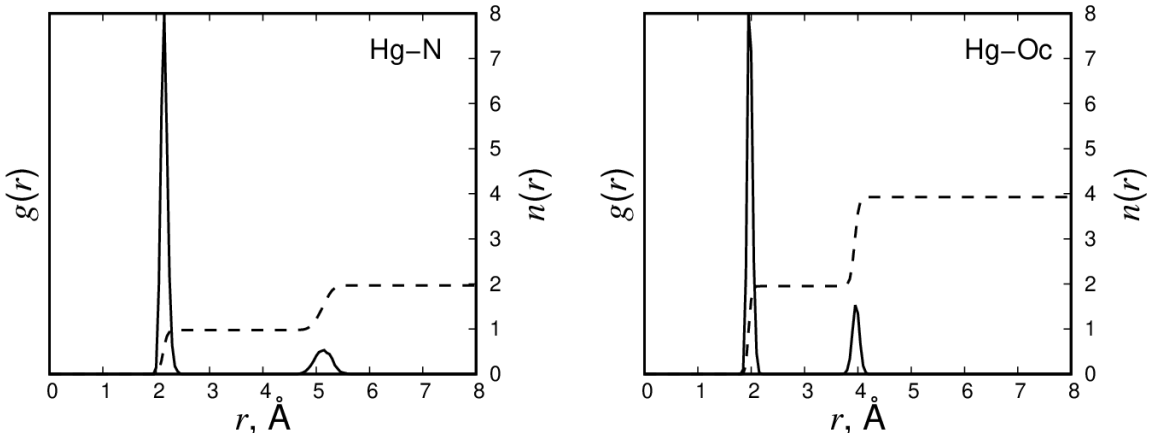


Figure S4. The radial distribution functions *g(r)* (solid line) and running coordination functions *n(r)* (dashed line) for *th*EDTA$_a^{2-}$+Hg^{2+}.

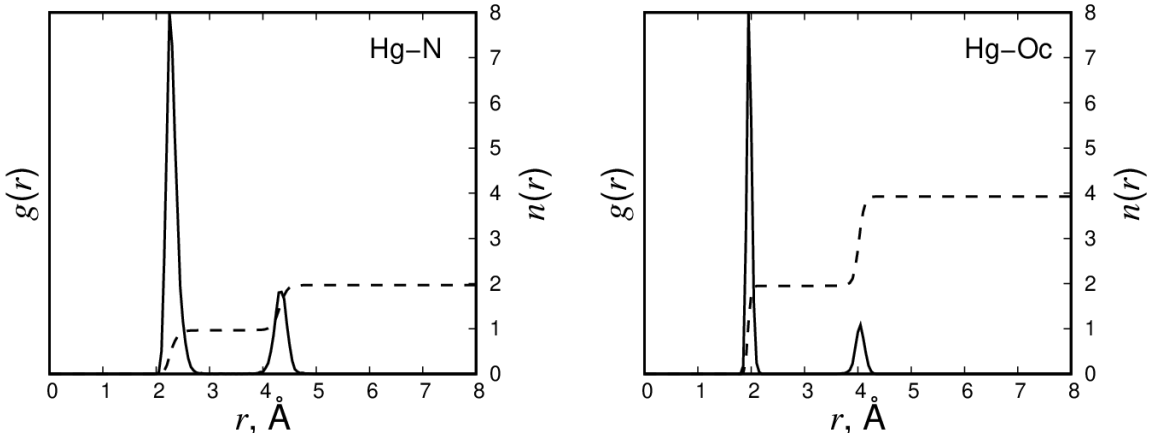


Figure S5. The radial distribution functions *g(r)* (solid line) and running coordination functions *n(r)* (dashed line) for *th*EDTA$_o^{2-}$+Hg^{2+}.

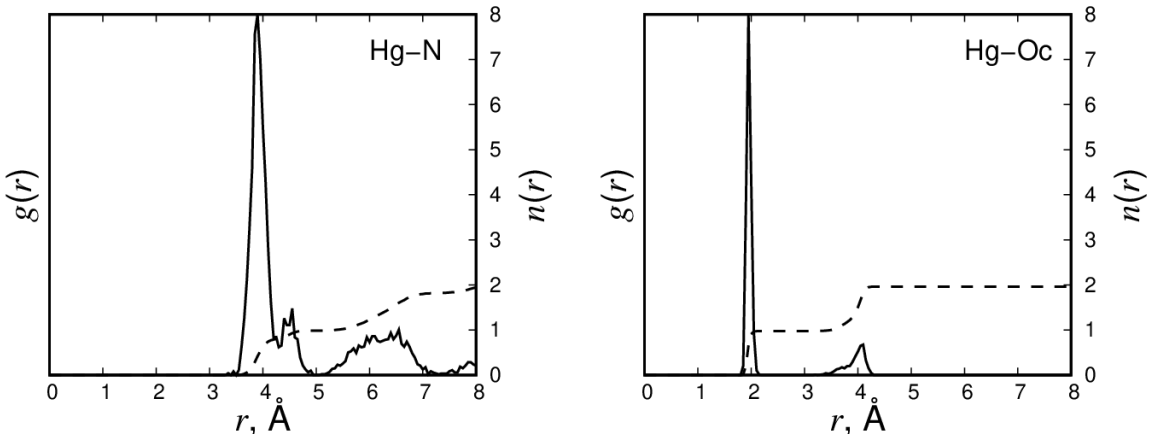


Figure S6. The radial distribution functions *g(r)* (solid line) and running coordination functions *n(r)* (dashed line) for *th*EDTA^{1-}+Hg^{2+}.

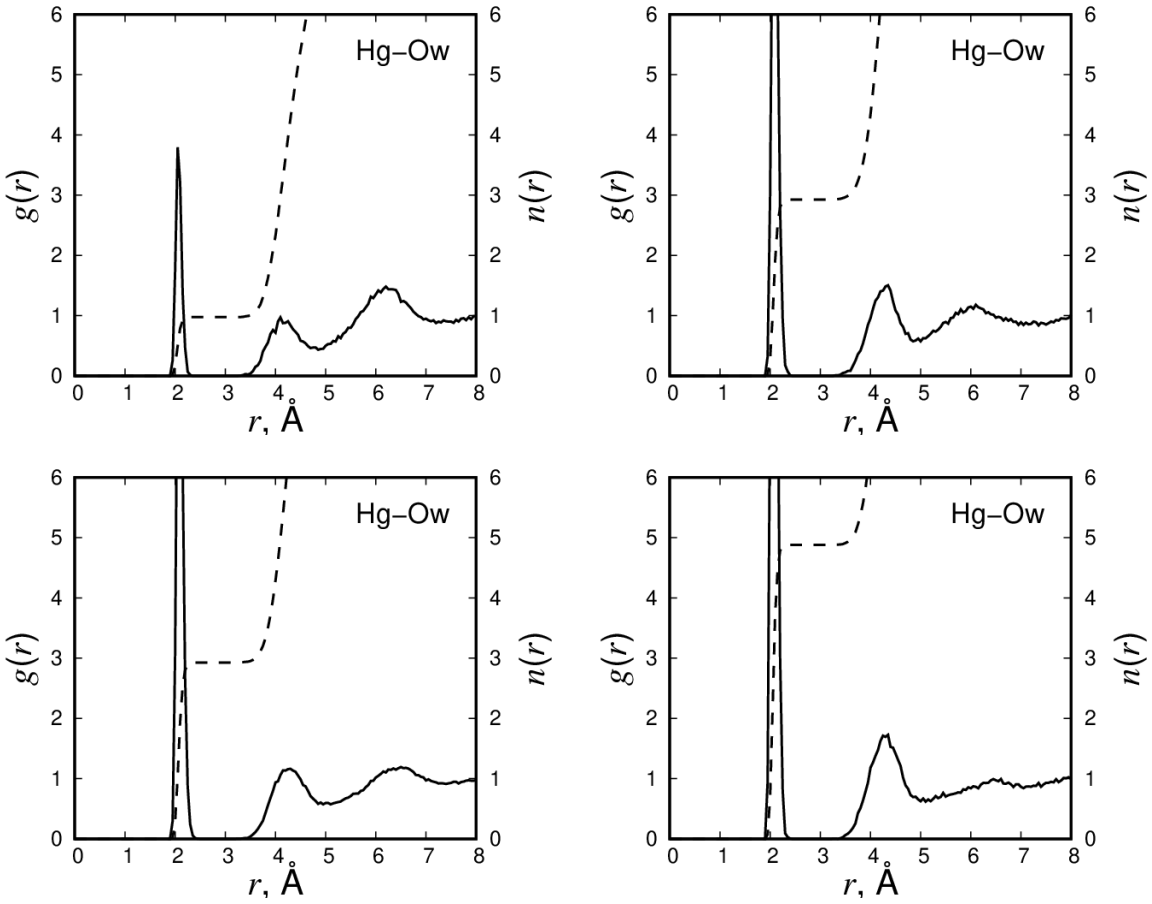
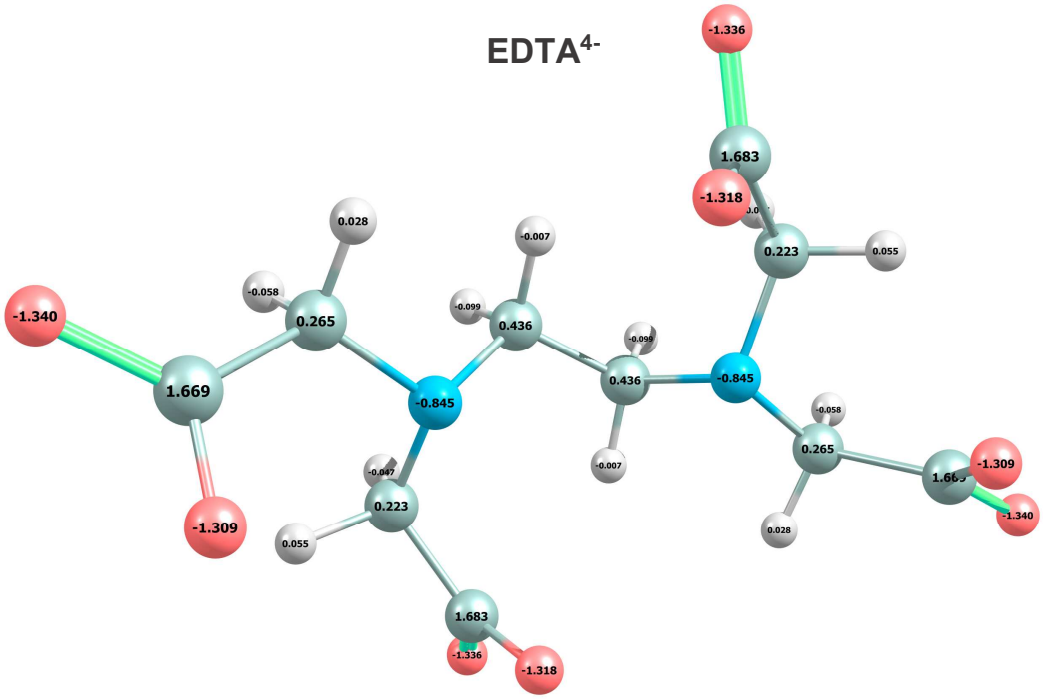
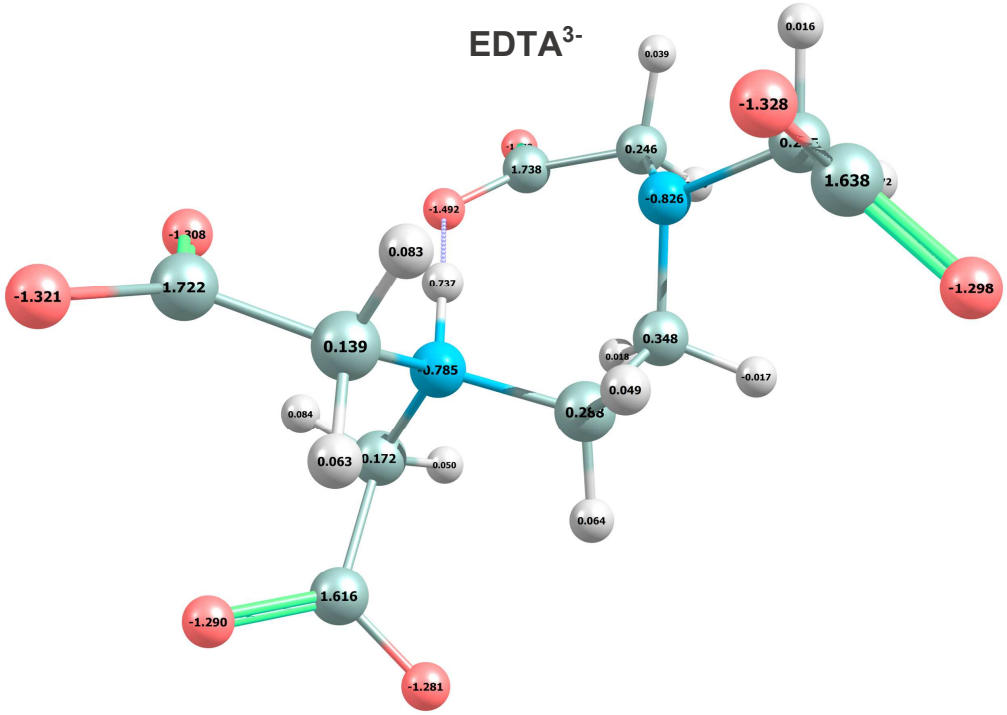
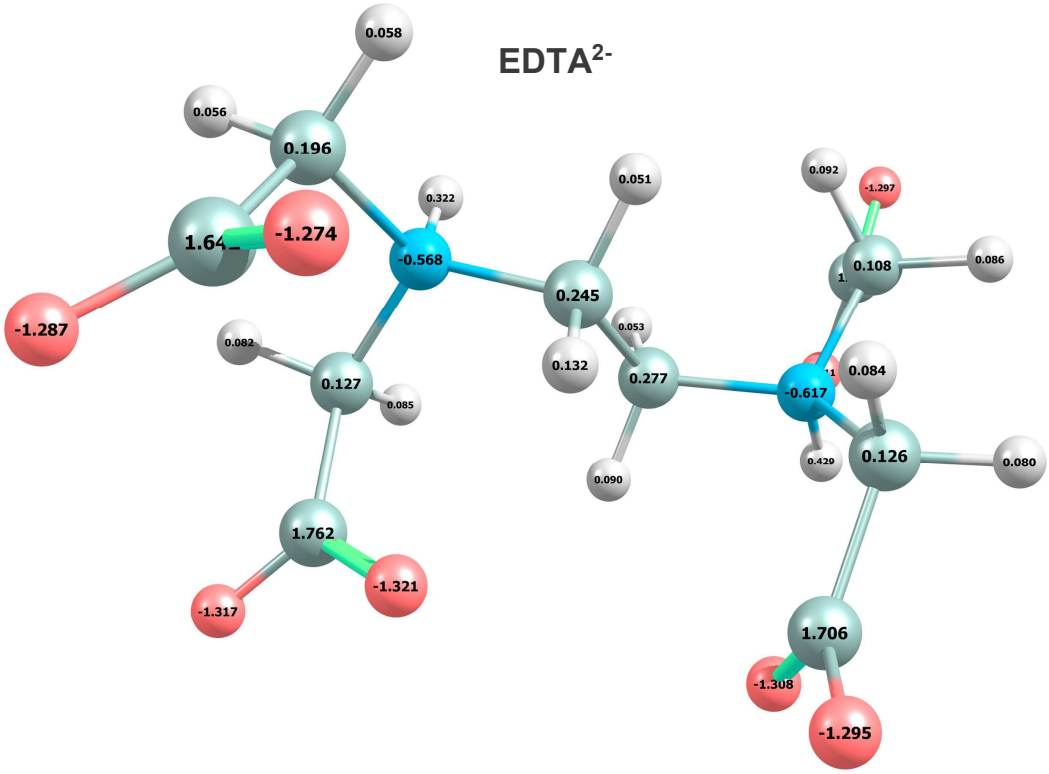
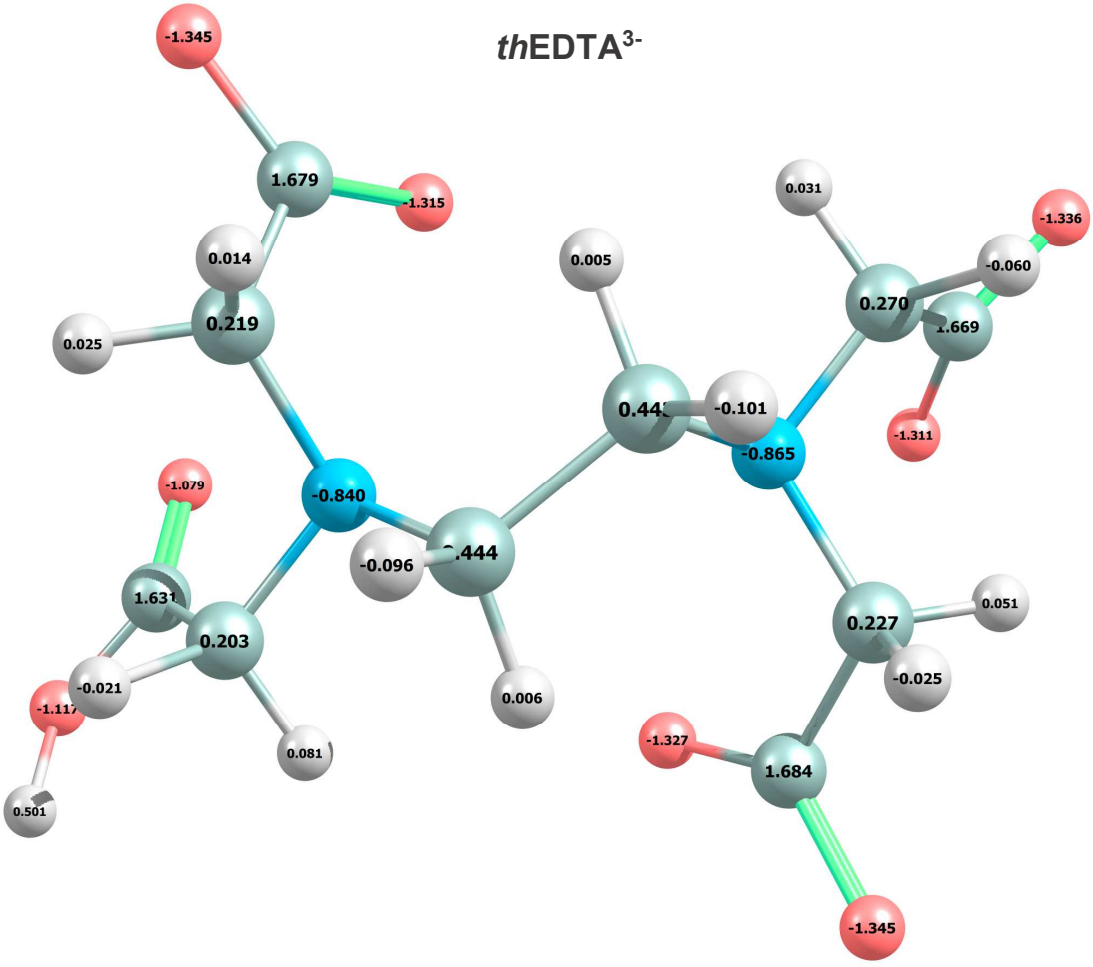


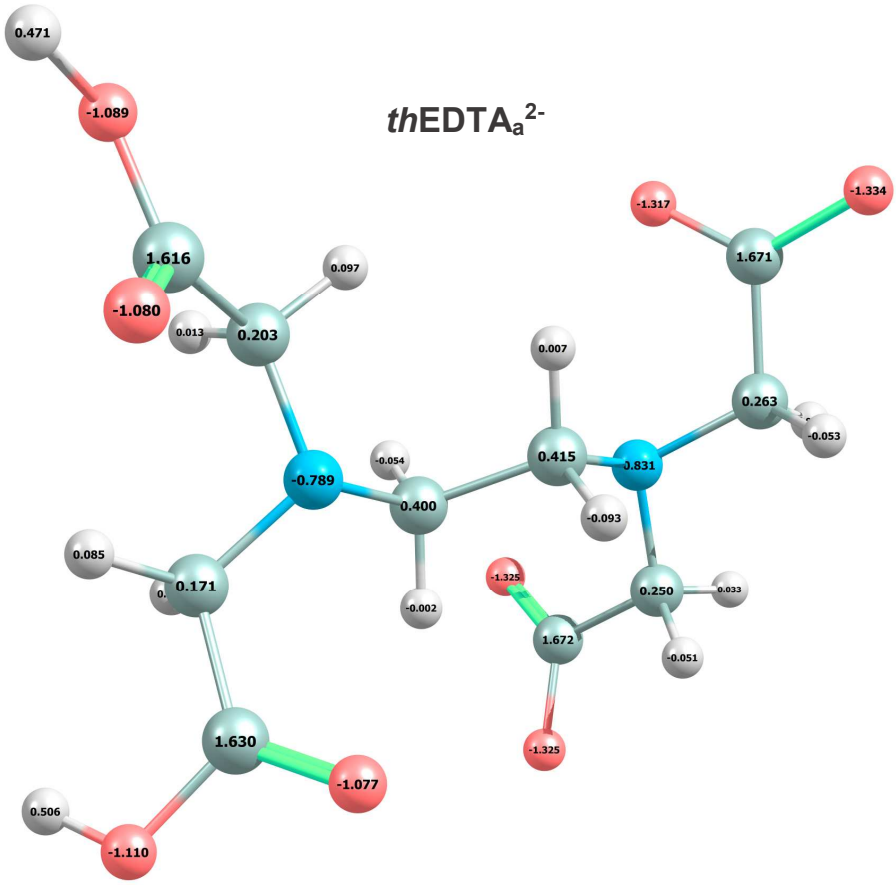
Figure S7. The radial distribution functions g(r) (solid line) and running coordination functions n(r) (dashed line) of Hg^{2+}-Ow in the different complexes of *th*EDTA+Hg^{2+}.

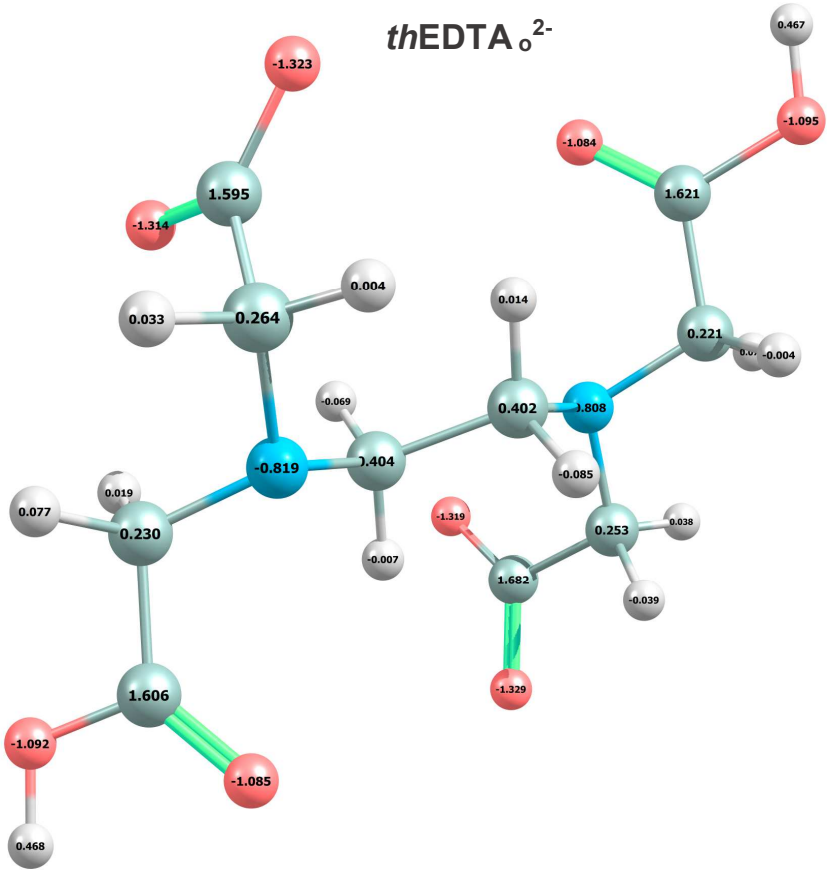

EDTA4-
-1.336
1.683
-1.318
0.028
-0.007
0.223
0.055
-0.058
-1.340
0.265
-0.099
0.436
-0.099
1.669
-0.845
0.436
-0.845
-0.058
0.265
-1.309
-0.007
-0.047
0.223
-1.309
0.055
0.028
1.683
-1.336
-1.318


EDTA3-
0.016
0.039
-1.328
0.246
1.738
1.638
-1.492
-0.826
-1.308
0.083
-1.321
1.722
0.737
-1.298
0.139
0.348
0.018
-0.785
-0.017
0.049
0.084
0.288
0.063
0.172
0.050
0.064
1.616
-1.290
-1.281


EDTA2-
0.058
0.056
0.196
1.64_
-1.274
-1.287
0.322
-0.568
0.051
0.245
0.053
0.132
0.277
0.082
0.127
0.085
1.762
-1.317
-1.321
0.092
-1.297
0.108
0.086
-0.617
0.084
0.420
0.126
0.080
0.090
1.706
-1.308
-1.295


thEDTA3-
-1.345
1.679
-1.315
0.014
0.219
0.025
0.005
0.031
-1.336
-0.060
0.270
1.669
-1.311
0.44_
-0.101
-0.865
-1.079
-0.840
-0.096
.444
1.631
0.203
-0.021
-1.117
0.501
0.081
0.006
0.227
0.051
-0.025
-1.327
1.684
-1.345


thEDTA$_a^{2-}$
0.471
-1.089
1.616
-1.080
0.013
0.203
0.097
-1.317
-1.334
1.671
0.007
0.263
-0.053
-0.054
-0.789
0.400
0.415
-0.831
-0.093
0.085
0.171
-1.325
0.250
0.033
1.672
-0.051
-0.002
-1.325
1.630
-1.077
0.506
-1.110


thEDTA $_o^{2-}$
-1.323
1.595
-1.314
0.033
0.264
0.004
0.467
-1.095
-1.084
1.621
0.014
0.221
-0.004
-0.069
0.402
-0.819
0.404
-0.085
0.019
0.077
0.230
-1.319
0.253
0.038
-0.007
1.682
-0.039
-1.329
1.606
-1.092
-1.085
0.468

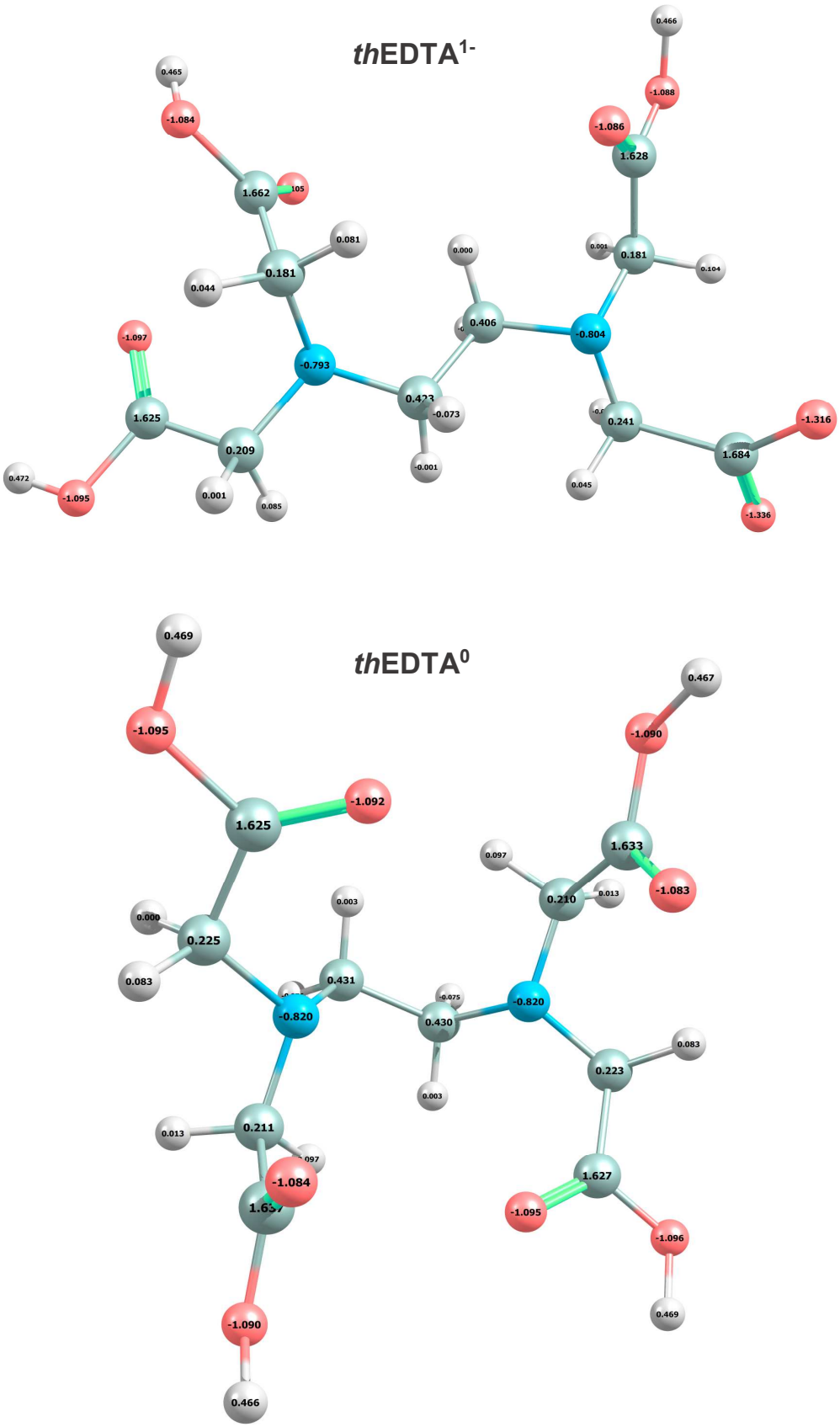
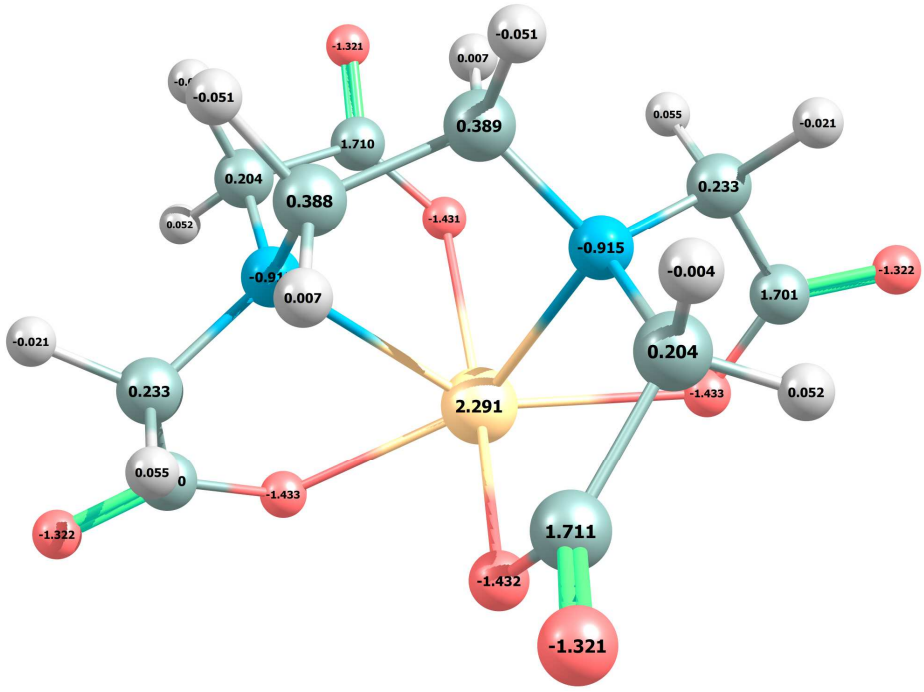
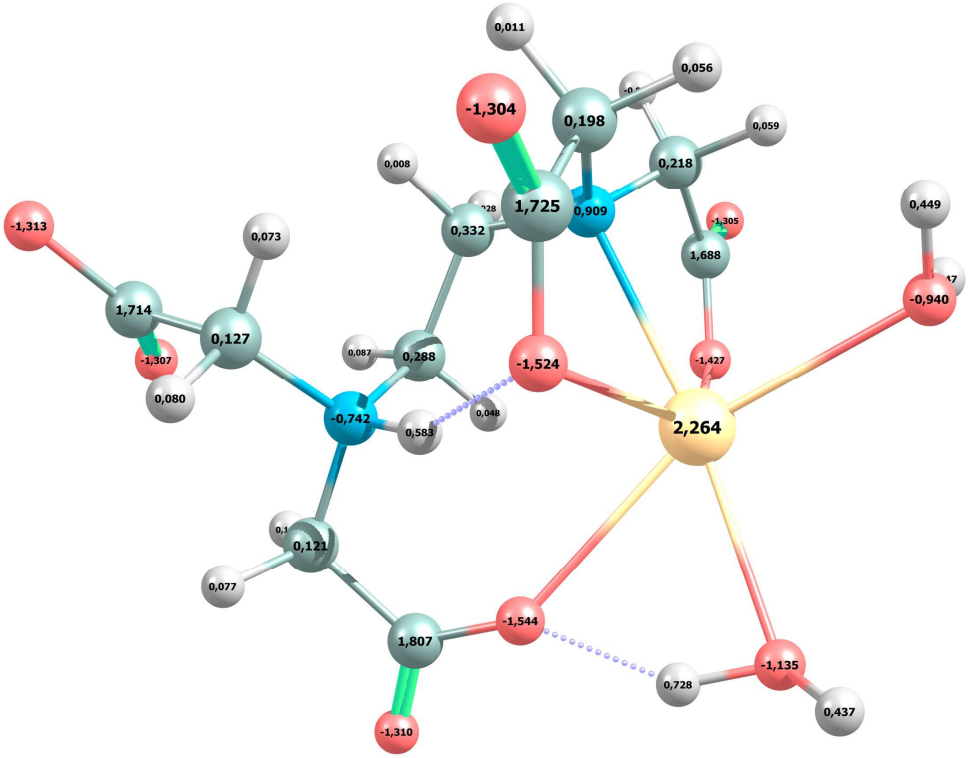


Figure S8. The APT partial charges of EDTA at different protonation states. The grey, red, blue, white, and yellow balls represent the carbon, oxygen, nitrogen, hydrogen, and mercury atoms, respectively.

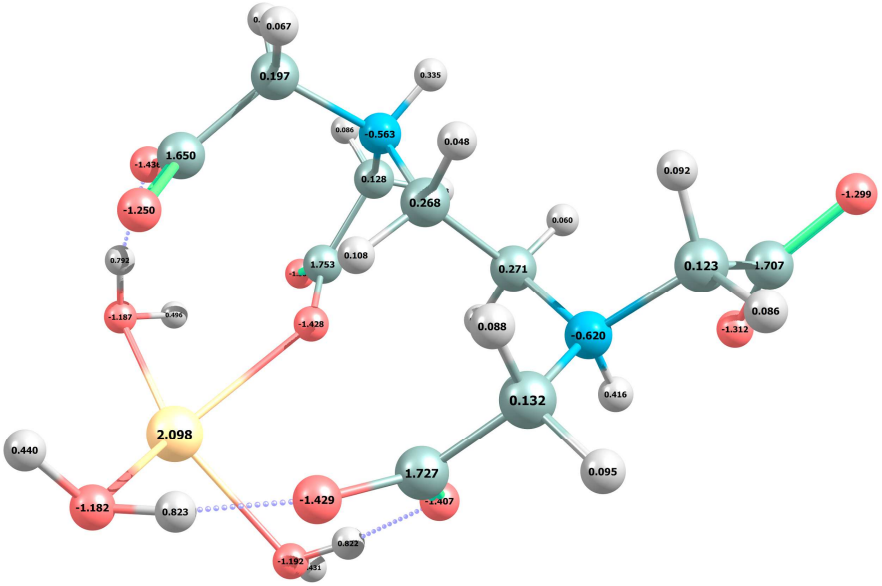
$EDTA^{4-}/Hg^{2+}$



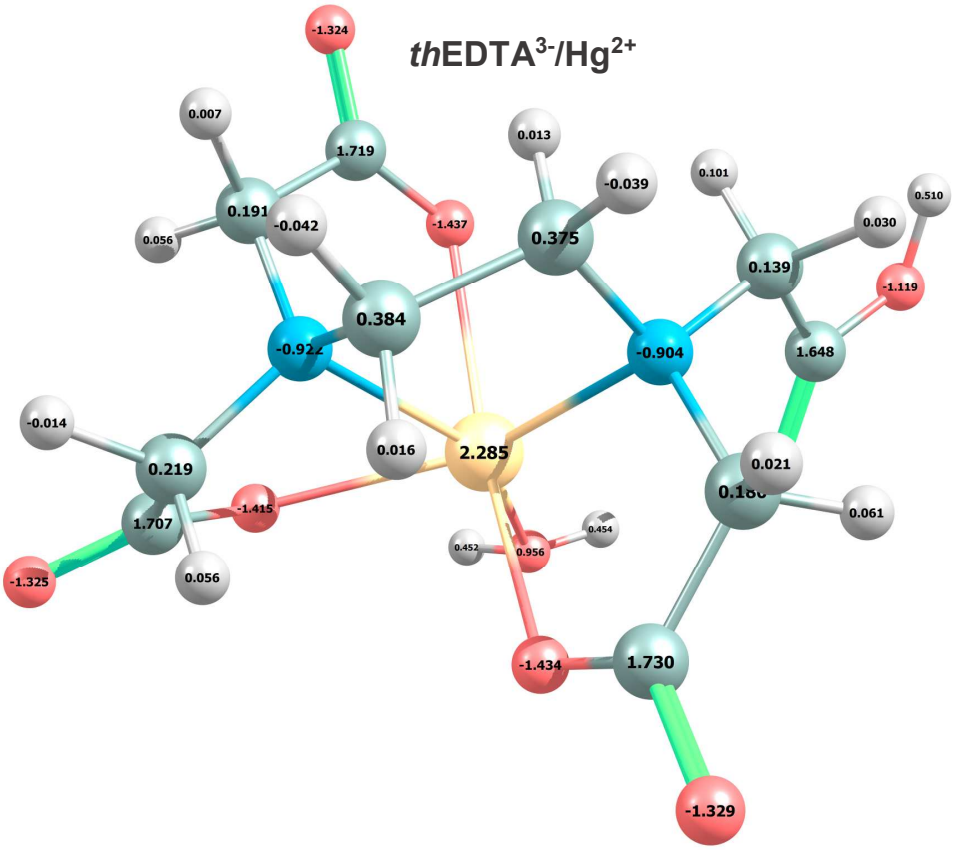
$EDTA^{3-}/Hg^{2+}$



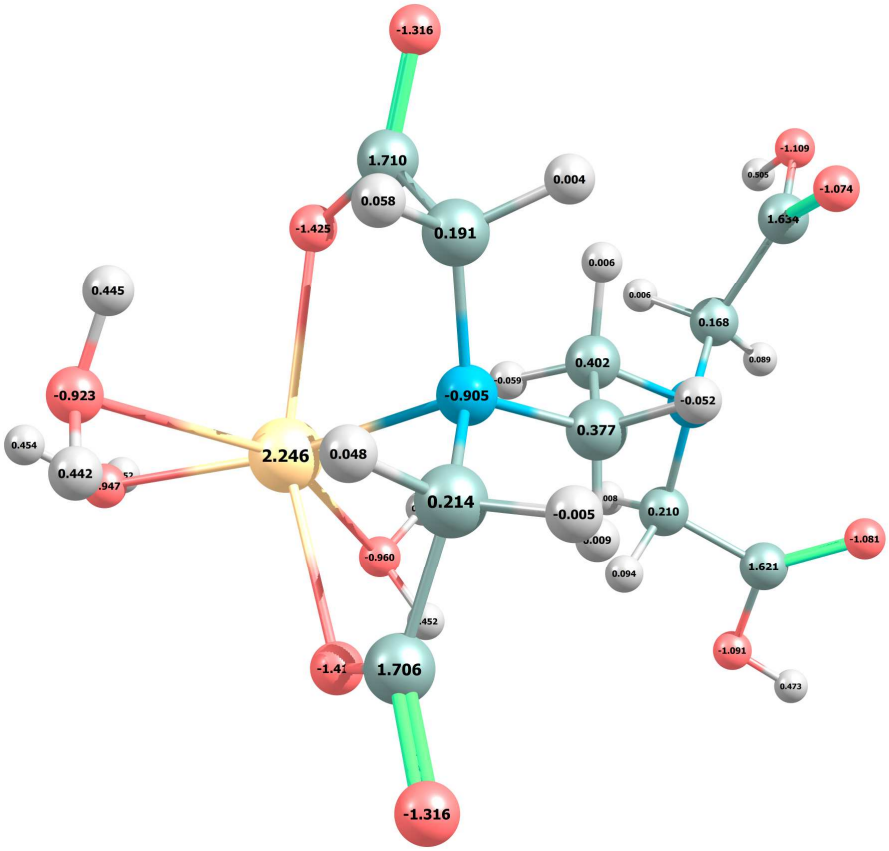
$EDTA^{2-}/Hg^{2+}$



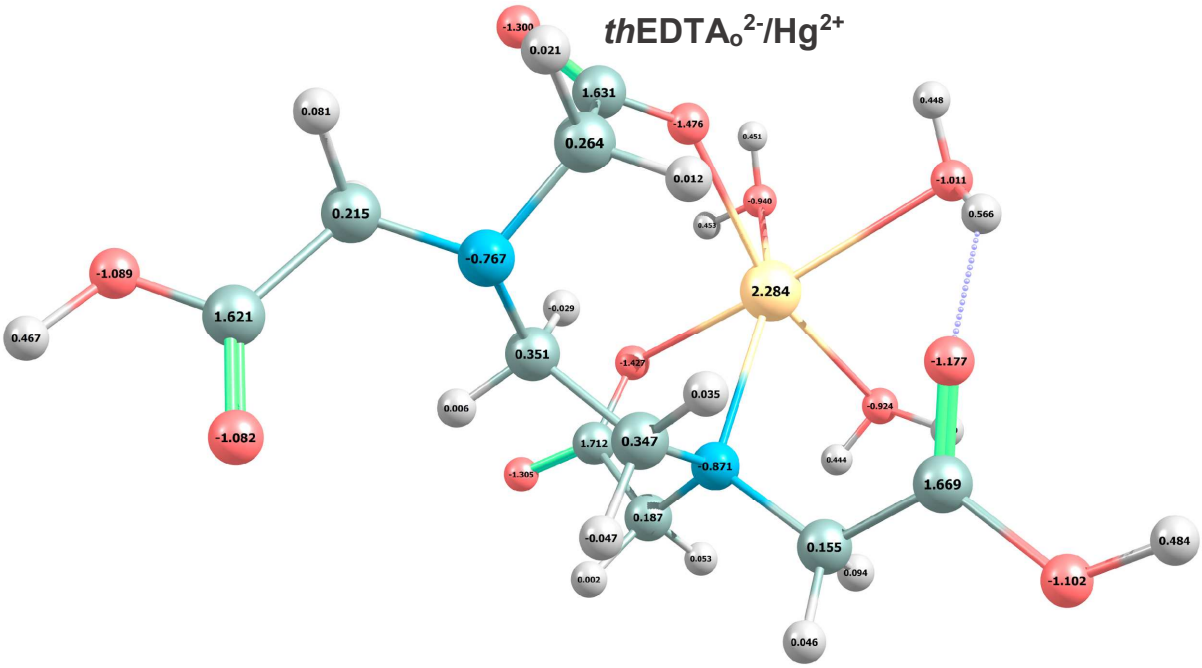
th$EDTA^{3-}/Hg^{2+}$



*th*EDTA$_a^{2-}$/Hg^{2+}



*th*EDTA$_o^{2-}$/Hg^{2+}



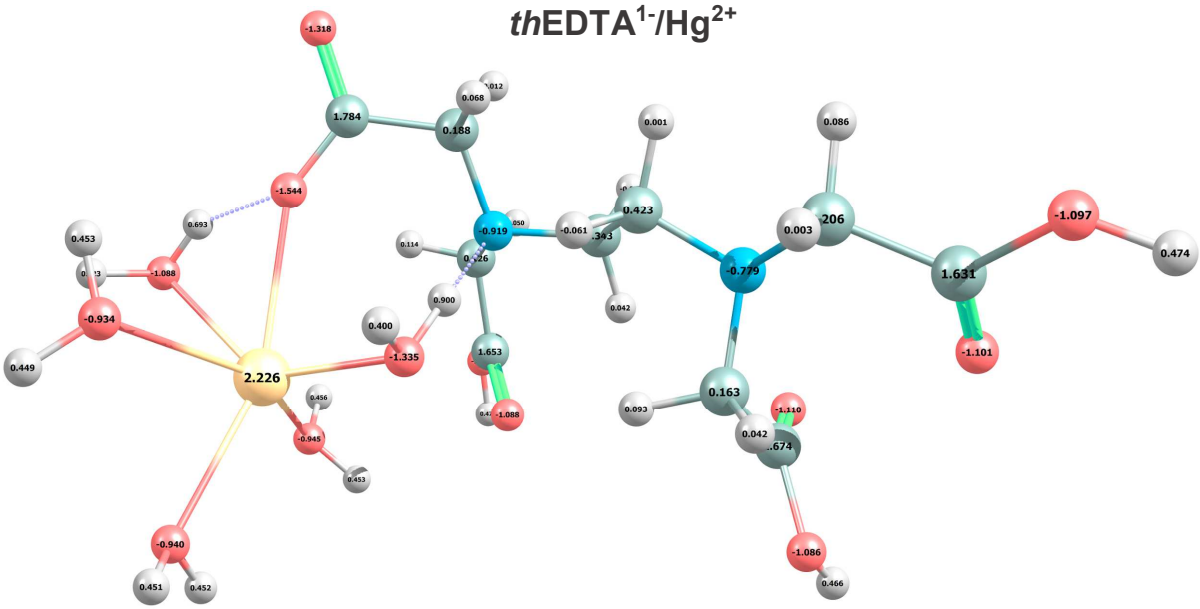


Figure S9. The APT partial charges of the EDTA-Hg^{2+} complexes at different protonation states. The grey, red, blue, white, and yellow balls represent the carbon, oxygen, nitrogen, hydrogen, and mercury atoms, respectively.

Atomic coordinates

The atomic coordinates of EDTA and the EDTA-Hg^{2+} complexes optimized at different protonation states and the M05-2X/LanL2DZ/SMD computational level are as follows.

$EDTA^{4-}$

```
O      1.371805 3.649116 -0.781571
O      4.855611 -1.479683 0.604243
O      -1.369595 -3.648520 -0.782307
O      -4.856097 1.479307 0.604106
O      0.781509 2.431556 1.054558
O      3.514692 -0.039794 1.761314
O      -0.782042 -2.431373 1.054973
O      -3.515164 0.039390 1.761110
N      1.643559 0.026335 -0.395932
N      -1.643784 -0.026286 -0.395950
C      0.655223 -0.390978 -1.422953
C      -0.655457 0.391259 -1.422877
C      2.154094 1.380658 -0.678342
C      2.746541 -0.950343 -0.383249
C      -2.154027 -1.380728 -0.678444
C      -2.746964 0.950158 -0.383355
C      1.358357 2.547335 -0.093637
C      3.763555 -0.790510 0.743719
C      -1.357805 -2.547086 -0.093790
C      -3.764005 0.790179 0.743569
H      1.104251 -0.275567 -2.424866
H      0.454825 -1.456460 -1.293607
H      -0.455042 1.456702 -1.293234
H      -1.104482 0.276073 -2.424817
H      2.250693 1.550639 -1.760208
H      3.154026 1.477031 -0.246122
H      3.309851 -0.945379 -1.330051
H      2.324069 -1.953670 -0.271196
H      -2.250612 -1.550649 -1.760315
H      -3.153894 -1.477339 -0.246140
H      -3.310237 0.945038 -1.330181
H      -2.324706 1.953577 -0.271344
```

$EDTA^{3-}$

```
O      -3.96561 -0.54137 -0.83870
O      -2.17651  1.38491  1.83289
O      1.94030  3.87040 -0.27963
O      2.90630 -3.07956 -0.34874
O      -2.69123 -1.06480 -2.66370
O      -3.18913 -0.51728  2.60839
O      0.35126  2.31481  0.21224
O      2.05933 -2.30704  1.62751
```

N	-0.84476	-0.03481	-0.17348
N	2.13647	0.21412	-0.07481
C	0.10975	-0.94051	-0.93167
C	1.37282	-0.16632	-1.28916
C	-1.85344	0.59377	-1.10952
C	-1.46244	-0.76721	0.97836
C	2.65407	1.58712	-0.14575
C	3.23365	-0.74261	0.19832
C	-2.91030	-0.41348	-1.57142
C	-2.35175	0.10902	1.85349
C	1.57042	2.65489	-0.06988
C	2.69610	-2.13850	0.51363
H	0.34017	-1.79214	-0.29563
H	-0.39717	-1.30126	-1.82580
H	1.98235	-0.78703	-1.95792
H	1.10165	0.73254	-1.84946
H	-1.29431	0.97530	-1.96212
H	-2.32694	1.41197	-0.57515
H	-0.64413	-1.13670	1.60110
H	-2.02278	-1.62268	0.60545
H	3.23774	1.77187	-1.05950
H	3.32276	1.76144	0.70148
H	3.78903	-0.39061	1.06976
H	3.91715	-0.81260	-0.65784
H	-0.27830	0.79709	0.18311

EDTA^{2-}

O	-1.97107	1.18939	0.69108
O	-2.90677	-0.02958	-2.22831
O	4.65006	-2.25226	-0.16827
O	1.26150	2.68631	0.91975
O	-3.03335	0.47625	2.58594
O	-4.26925	-0.63590	-0.48946
O	3.96795	-0.67566	1.35562
O	0.25964	3.38519	-1.02262
N	-1.19979	-1.57730	0.08620
N	2.09929	0.35178	-0.19961
C	-0.17820	-0.66186	-0.55697
C	0.91820	-0.33490	0.45652
C	-1.75648	-1.13946	1.42748
C	-2.29162	-1.95074	-0.90116
C	3.02208	-0.63517	-0.85947
C	1.70647	1.47647	-1.11542
C	-2.30048	0.28661	1.54280
C	-3.21983	-0.77367	-1.22461
C	3.94632	-1.24296	0.19649
C	1.00548	2.59201	-0.34054
H	0.20993	-1.21023	-1.41604
H	-0.70263	0.22659	-0.88536
H	0.55319	0.34245	1.22448

H	1.30381	-1.23916	0.93051
H	-0.96134	-1.25324	2.16588
H	-2.55056	-1.84033	1.67879
H	-2.85952	-2.75866	-0.44518
H	-1.79362	-2.29705	-1.80416
H	3.63118	-0.11557	-1.59945
H	2.44827	-1.41143	-1.36024
H	1.09109	1.09984	-1.92766
H	2.62293	1.89042	-1.53934
H	-0.70816	-2.46016	0.28398
H	2.63757	0.75735	0.58712

***th*EDTA^{3-}**

O	2.419931	3.498741	-0.443891
O	4.458499	-2.135015	0.846343
O	-1.021463	-2.347542	0.782835
O	-4.335917	1.981028	1.036527
O	0.997513	2.322779	0.895537
O	3.411086	-0.314823	1.741028
O	-2.681817	-3.384018	-0.389542
O	-3.349734	0.041929	1.598832
N	1.677582	-0.129200	-0.512024
N	-1.556950	0.137249	-0.603738
C	0.686835	-0.419977	-1.574843
C	-0.512780	0.523526	-1.582337
C	2.384214	1.135727	-0.763940
C	2.607127	-1.260852	-0.377941
C	-2.234385	-1.116501	-0.973446
C	-2.490060	1.237694	-0.370239
C	1.874963	2.386795	-0.045557
C	3.546939	-1.210016	0.823682
C	-1.943214	-2.349287	-0.114886
C	-3.387061	1.005479	0.820865
H	1.174750	-0.364853	-2.562768
H	0.335807	-1.446491	-1.447148
H	-0.185703	1.541193	-1.361850
H	-0.938645	0.532449	-2.598477
H	2.402035	1.374539	-1.837490
H	3.428968	1.040036	-0.456220
H	3.239032	-1.388602	-1.271697
H	2.026043	-2.181344	-0.268762
H	-1.984748	-1.398881	-2.005118
H	-3.320601	-0.986837	-0.959498
H	-3.143938	1.444323	-1.233906
H	-1.930977	2.156780	-0.168341
H	-4.326699	2.721175	0.392123

***th*EDTA$_a^{2-}$**

O	-1.896485	-2.343453	1.990758
O	-4.028746	2.744879	-1.207859
O	3.712032	-2.671437	-0.541036
O	2.877465	3.541691	1.019093
O	-1.380537	-3.772796	0.288436
O	-2.891298	2.428091	0.744666
O	2.031758	-1.814790	-1.762272
O	3.305448	2.259210	-0.821254
N	-2.257890	-0.251895	-0.020504
N	1.511645	0.245365	0.123191
C	-0.905427	0.215351	-0.404626
C	0.207907	-0.392781	0.445448
C	-2.419629	-1.689890	-0.307070
C	-3.268641	0.524744	-0.759106
C	2.636983	-0.667996	0.329297
C	1.691393	1.491118	0.873647
C	-1.842521	-2.646926	0.737114
C	-3.379617	1.997654	-0.368041
C	2.731081	-1.726631	-0.743727
C	2.694270	2.422197	0.247623
H	-0.707748	-0.024735	-1.463117
H	-0.883309	1.300961	-0.299083
H	-0.023557	-0.281181	1.513183
H	0.297258	-1.460224	0.236138
H	-1.987852	-1.955168	-1.282977
H	-3.489081	-1.919121	-0.350372
H	-4.255958	0.090499	-0.578070
H	-3.095633	0.491063	-1.845909
H	2.591894	-1.182020	1.302102
H	3.583040	-0.119402	0.305847
H	2.000248	1.320341	1.915303
H	0.746054	2.037042	0.916335
H	4.224783	-2.572288	0.290400
H	3.511679	4.187744	0.633810

***th*EDTA$_o^{2-}$**

O	-4.866644	0.173233	0.206549
O	-0.884458	-2.791748	1.589285
O	-0.731364	3.863765	0.281694
O	4.911866	-0.433274	-0.751248
O	-3.413260	0.997944	-1.348390
O	0.835378	-3.598225	0.319132
O	0.130359	2.542515	1.931003
O	3.324735	-1.038579	0.775855
N	-1.489338	-0.989661	-0.643465
N	1.641199	1.112564	-0.104371
C	-0.598372	0.007771	-0.007162

C	0.742595	0.111511	-0.729040
C	-2.806837	-0.989465	-0.010389
C	-0.888287	-2.324179	-0.802155
C	1.144930	2.487123	-0.297452
C	2.999910	0.962588	-0.635478
C	-3.673033	0.154183	-0.474726
C	-0.267477	-2.935919	0.461855
C	0.103461	2.969908	0.714851
C	3.707425	-0.261648	-0.113920
H	-1.116849	0.968131	-0.042593
H	-0.420889	-0.239934	1.049562
H	1.248947	-0.853616	-0.691501
H	0.572178	0.364766	-1.788402
H	-2.763155	-0.931356	1.085179
H	-3.345239	-1.908919	-0.253842
H	-0.121343	-2.295765	-1.575458
H	-1.664726	-3.012639	-1.147627
H	0.723592	2.623584	-1.302647
H	1.983026	3.183800	-0.199591
H	3.615178	1.815969	-0.339044
H	3.028741	0.913251	-1.734236
H	-5.470721	0.897576	-0.073082
H	5.429437	-1.201453	-0.421202

***th*EDTA^{1-}**

O	3.254628	3.159199	-0.531960
O	4.553941	-2.936138	-0.476839
O	-3.352076	2.577704	0.577237
O	-4.937517	-2.397065	0.111385
O	1.966924	2.326339	1.159152
O	4.485767	-1.252142	1.062780
O	-2.181245	1.898483	-1.258952
O	-4.405726	-0.307783	-0.646618
N	2.046245	-0.275312	-0.035136
N	-1.717196	-0.638354	0.102831
C	0.630491	-0.130957	-0.455840
C	-0.312813	-1.068054	0.299116
C	2.844630	0.823436	-0.588216
C	2.595019	-1.571743	-0.467648
C	-2.050197	0.595796	0.826405
C	-2.672388	-1.717145	0.365523
C	2.617217	2.131566	0.118615
C	3.975488	-1.920462	0.085472
C	-2.519714	1.706461	-0.079005
C	-4.054947	-1.374973	-0.115010
H	0.332237	0.901263	-0.262899
H	0.527144	-0.304420	-1.538868
H	-0.222806	-2.087030	-0.079533
H	-0.047890	-1.077535	1.366276

H	2.653221	0.987829	-1.659381
H	3.908981	0.600798	-0.484067
H	2.651947	-1.642696	-1.564675
H	1.930094	-2.370370	-0.132035
H	-1.173804	0.985357	1.358602
H	-2.818311	0.432633	1.587162
H	-2.751666	-1.973878	1.432790
H	-2.361785	-2.622479	-0.160410
H	3.156021	4.029709	-0.085208
H	-3.626616	3.346925	0.029619
H	-5.854407	-2.202773	-0.187201

***th*EDTA^0**

O	-0.245684	-4.127276	-0.549569
O	4.371483	0.491107	-0.284333
O	0.217497	4.144788	-0.545627
O	-4.358660	-0.508520	-0.280891
O	0.690913	-2.402387	-1.716902
O	2.260930	1.315268	-0.568800
O	-0.705337	2.413791	-1.714806
O	-2.244526	-1.326513	-0.557054
N	1.167369	-0.988122	0.713708
N	-1.161646	0.988205	0.713616
C	0.747661	-0.178919	1.875928
C	-0.737977	0.183613	1.877849
C	0.672362	-2.360241	0.746760
C	2.600068	-0.907316	0.449866
C	-0.675192	2.363604	0.748571
C	-2.594119	0.899636	0.449927
C	0.391200	-2.913399	-0.625929
C	3.005499	0.402784	-0.177357
C	-0.406267	2.924238	-0.623598
C	-2.993219	-0.414867	-0.171876
H	0.963834	-0.703755	2.820045
H	1.349309	0.732162	1.880628
H	-1.339982	-0.727005	1.889518
H	-0.950605	0.713063	2.820135
H	-0.262723	-2.412956	1.304889
H	1.365810	-3.058354	1.240194
H	2.898283	-1.690818	-0.252040
H	3.213051	-1.041331	1.353423
H	0.262922	2.420309	1.301525
H	-1.370430	3.055260	1.248780
H	-2.895370	1.678569	-0.255704
H	-3.208034	1.035082	1.352676
H	-0.428851	-4.532807	-1.426536
H	4.683607	1.323441	-0.705361
H	0.393536	4.555366	-1.421774
H	-4.667440	-1.343647	-0.698662

$EDTA^{4-}/Hg^{2+}$

O	1.407914	-3.683953	1.241244
O	4.248397	1.329597	-0.831786
O	-1.401187	3.682094	1.245702
O	-4.256319	-1.311133	-0.829421
O	0.486718	-2.308659	-0.321485
O	2.252344	0.486338	-1.529919
O	-0.486357	2.306918	-0.320874
O	-2.253302	-0.486832	-1.530116
N	1.522238	-0.026090	1.148895
N	-1.521254	0.024328	1.149802
C	0.673643	0.358949	2.303623
C	-0.672211	-0.364845	2.302822
C	2.088876	-1.382785	1.284781
C	2.564556	0.972695	0.847480
C	-2.085079	1.381839	1.289288
C	-2.565880	-0.971849	0.847313
C	1.251390	-2.525977	0.705853
C	3.058567	0.910108	-0.598718
C	-1.247679	2.524362	0.708883
C	-3.062162	-0.903419	-0.597870
H	1.186539	0.132451	3.248252
H	0.514368	1.439268	2.271974
H	-0.513206	-1.445073	2.267409
H	-1.184582	-0.141312	3.248452
H	2.298812	-1.617598	2.334160
H	3.041767	-1.425381	0.746194
H	3.433339	0.877268	1.508522
H	2.148675	1.974676	0.986135
H	-2.291046	1.615695	2.339656
H	-3.039788	1.426819	0.754083
H	-3.433193	-0.876901	1.510286
H	-2.151169	-1.974866	0.981918
Hg	-0.000340	-0.001027	-0.872943

$EDTA^{3-}/Hg^{2+}$

O	-0.38411	0.54628	-0.74826
O	-1.03288	1.31044	2.24576
O	6.83493	0.25405	-0.41389
O	1.10453	-2.25481	-0.47068
O	-1.09718	2.04228	-2.32026
O	-1.82443	2.86007	0.76445
O	5.22735	-0.71868	-1.73496
O	0.42200	-2.19746	1.71163
N	1.39002	2.48249	0.38655
N	3.39592	-0.80386	0.16751
C	1.90896	1.11901	0.81667
C	2.64703	0.42438	-0.32617
C	0.81217	2.62805	-1.01021

C	0.47058	3.04540	1.46085
C	4.78910	-0.44898	0.61669
C	2.67921	-1.58911	1.23104
C	-0.31999	1.67401	-1.37247
C	-0.88970	2.33751	1.49731
C	5.68551	-0.28106	-0.61026
C	1.29549	-2.03743	0.78350
H	2.57292	1.31882	1.65915
H	1.05410	0.54541	1.15547
H	1.94921	0.08682	-1.08680
H	3.38767	1.08372	-0.77992
H	1.62596	2.48995	-1.72335
H	0.45850	3.65447	-1.09372
H	0.33131	4.10035	1.23718
H	0.98348	2.92091	2.41187
H	5.18151	-1.26286	1.22706
H	4.76215	0.46206	1.21104
H	2.61441	-0.99634	2.13944
H	3.27633	-2.47851	1.43884
H	2.21014	3.10559	0.38356
H	3.51463	-1.40131	-0.66818
Hg	-2.36822	-0.66485	-0.25836
O	-2.12957	-1.78228	1.81687
H	-2.33292	-1.18443	2.55970
H	-1.14719	-2.01835	1.78825
O	-3.40972	1.42189	-0.68756
H	-2.90007	2.00404	-0.02787
H	-3.04774	1.60203	-1.58314
O	-1.35496	-2.56498	-1.25849
H	-1.47988	-2.66001	-2.21992
H	-0.37660	-2.50015	-0.99691

$EDTA^{2-}/Hg^{2+}$

O	-0.38411	0.54628	-0.74826
O	-1.03288	1.31044	2.24576
O	6.83493	0.25405	-0.41389
O	1.10453	-2.25481	-0.47068
O	-1.09718	2.04228	-2.32026
O	-1.82443	2.86007	0.76445
O	5.22735	-0.71868	-1.73496
O	0.42200	-2.19746	1.71163
N	1.39002	2.48249	0.38655
N	3.39592	-0.80386	0.16751
C	1.90896	1.11901	0.81667
C	2.64703	0.42438	-0.32617
C	0.81217	2.62805	-1.01021
C	0.47058	3.04540	1.46085
C	4.78910	-0.44898	0.61669
C	2.67921	-1.58911	1.23104
C	-0.31999	1.67401	-1.37247

C	-0.88970	2.33751	1.49731
C	5.68551	-0.28106	-0.61026
C	1.29549	-2.03743	0.78350
H	2.57292	1.31882	1.65915
H	1.05410	0.54541	1.15547
H	1.94921	0.08682	-1.08680
H	3.38767	1.08372	-0.77992
H	1.62596	2.48995	-1.72335
H	0.45850	3.65447	-1.09372
H	0.33131	4.10035	1.23718
H	0.98348	2.92091	2.41187
H	5.18151	-1.26286	1.22706
H	4.76215	0.46206	1.21104
H	2.61441	-0.99634	2.13944
H	3.27633	-2.47851	1.43884
H	2.21014	3.10559	0.38356
H	3.51463	-1.40131	-0.66818
Hg	-2.36822	-0.66485	-0.25836
O	-2.12957	-1.78228	1.81687
H	-2.33292	-1.18443	2.55970
H	-1.14719	-2.01835	1.78825
O	-3.40972	1.42189	-0.68756
H	-2.90007	2.00404	-0.02787
H	-3.04774	1.60203	-1.58314
O	-1.35496	-2.56498	-1.25849
H	-1.47988	-2.66001	-2.21992
H	-0.37660	-2.50015	-0.99691

***th*EDTA^{3-}/Hg^{2+}**

O	1.608454	-3.822786	0.818733
O	4.350188	1.445630	-0.531479
O	-0.460390	2.309900	0.066847
O	-4.183887	-1.682706	-0.732305
O	0.449947	-2.275248	-0.379941
O	2.453188	0.478684	-1.350105
O	-1.670826	3.589650	1.507445
O	-2.868294	0.077132	-1.200929
N	1.591298	-0.160132	1.229991
N	-1.486080	-0.089965	1.275326
C	0.741397	0.114024	2.417546
C	-0.598327	-0.614571	2.353625
C	2.149732	-1.528229	1.230012
C	2.647118	0.855906	1.053726
C	-2.046441	1.237029	1.610707
C	-2.534793	-1.067831	0.946970
C	1.329247	-2.605275	0.516222
C	3.189786	0.916315	-0.373906
C	-1.327408	2.450244	1.020664
C	-3.173816	-0.817047	-0.398024
H	1.258331	-0.196482	3.334996

H	0.578263	1.192016	2.482289
H	-0.434494	-1.679450	2.180037
H	-1.095343	-0.514986	3.326924
H	2.333428	-1.876667	2.252635
H	3.116815	-1.519464	0.717231
H	3.490168	0.695177	1.735219
H	2.229317	1.843467	1.268439
H	-2.080665	1.378033	2.696821
H	-3.077978	1.305211	1.253403
H	-3.335192	-1.090733	1.700399
H	-2.102304	-2.071136	0.907720
H	-4.382026	-2.376960	-0.066648
Hg	0.081173	0.097858	-0.720537
O	-0.331231	0.480259	-3.059850
H	0.407592	0.266163	-3.659074
H	-1.172424	0.120359	-3.397271

***th*EDTA$_a^{2-}$/Hg^{2+}**

O	1.162417	-2.118130	-0.926018
O	2.028971	2.190321	3.321751
O	-5.123232	-2.674908	-0.774947
O	-3.874550	3.635604	-0.579490
O	0.292627	-3.974206	0.061243
O	1.935769	1.869039	1.068805
O	-4.032820	-2.198361	1.130977
O	-4.947260	2.019774	0.627380
N	0.608071	-0.591210	1.430320
N	-2.866629	0.158054	0.056146
C	-0.782011	-0.059183	1.374626
C	-1.532387	-0.489369	0.114347
C	0.640205	-2.067066	1.470190
C	1.330719	0.025576	2.562047
C	-3.812058	-0.623761	-0.745068
C	-2.777270	1.537576	-0.432889
C	0.685399	-2.753296	0.102886
C	1.780220	1.463023	2.294520
C	-4.298979	-1.862231	-0.030960
C	-3.974166	2.370715	-0.059169
H	-1.340065	-0.402728	2.256591
H	-0.715722	1.030826	1.418399
H	-0.945473	-0.250800	-0.784841
H	-1.686654	-1.570060	0.130280
H	-0.215311	-2.471522	2.022817
H	1.546877	-2.393025	1.988522
H	2.237563	-0.547370	2.771265
H	0.722273	0.027013	3.473825
H	-3.385928	-0.939294	-1.710175
H	-4.700260	-0.027726	-0.971877
H	-2.658873	1.596009	-1.525312

H	-1.908467	2.033173	0.004975
H	-5.296518	-2.371116	-1.692135
H	-4.627704	4.222843	-0.343018
Hg	1.752590	0.181218	-0.647131
O	0.384070	1.870453	-1.808074
H	-0.402527	1.500634	-2.251477
H	0.114697	2.539058	-1.149257
O	3.872535	-0.883578	0.435450
H	4.030172	-0.380340	1.256848
H	3.523044	-1.770595	0.646835
O	3.371627	0.604276	-2.364822
H	3.044896	0.721682	-3.275752
H	4.147379	0.013787	-2.342493

***th*EDTA$_o^{2-}$/Hg^{2+}**

O	-6.141378	0.039314	0.373140
O	-2.314602	-3.050351	-0.821268
O	-0.902220	1.064152	3.678267
O	2.554233	3.234261	-2.200335
O	-4.867592	1.805890	-0.312008
O	-0.217370	-2.167770	-0.828380
O	0.384665	-0.326903	2.414367
O	1.678060	1.129489	-2.192418
N	-2.748659	0.055123	-1.019415
N	0.359032	1.668008	0.306961
C	-1.912838	0.584687	0.085268
C	-0.935962	1.641522	-0.441104
C	-4.013036	-0.498182	-0.529331
C	-2.005764	-0.889099	-1.886258
C	0.146452	2.007949	1.738359
C	1.260966	2.663005	-0.308506
C	-5.000909	0.579697	-0.166149
C	-1.485515	-2.119802	-1.130999
C	-0.164888	0.824402	2.656418
C	1.816858	2.234520	-1.639932
H	-2.569470	1.028643	0.835372
H	-1.369384	-0.232682	0.578892
H	-0.704933	1.436850	-1.485312
H	-1.400099	2.635316	-0.387648
H	-3.898947	-1.145722	0.350387
H	-4.479421	-1.106498	-1.308213
H	-1.159238	-0.373557	-2.337896
H	-2.673098	-1.224999	-2.680666
H	-0.650903	2.750322	1.845430
H	1.066212	2.445963	2.137939
H	2.120543	2.840875	0.341317
H	0.757253	3.627705	-0.452764
H	-6.824152	0.707676	0.606278
H	2.971704	2.996530	-3.059318

Hg	1.330283	-0.617311	0.173496
O	2.721991	-1.388928	-1.741524
H	2.322022	-2.208680	-2.087306
H	2.461450	-0.612240	-2.281691
O	3.425379	0.522734	0.976374
H	3.108044	1.122479	1.679391
H	3.826201	1.038963	0.251093
O	2.135456	-2.673560	1.315985
H	1.720140	-2.654376	2.199077
H	1.795689	-3.428403	0.798923

***th*EDTA^{1-}/Hg^{2+}**

O	-0.770952	1.551831	3.423116
O	-1.733985	-4.055958	1.103625
O	4.519442	2.924315	-0.494111
O	7.150837	-1.389783	-1.673869
O	0.232251	1.759589	1.382378
O	-2.170793	-1.958622	0.340812
O	4.344543	1.769021	1.465683
O	6.512121	0.384782	-0.382335
N	0.422127	-1.079284	1.146549
N	3.906381	-0.640893	-0.133298
C	1.902015	-0.898295	1.280369
C	2.666285	-1.427614	0.060234
C	-0.268412	-0.468298	2.300831
C	0.097284	-2.526104	1.070922
C	3.640326	0.713626	-0.642433
C	4.886638	-1.360096	-0.952685
C	-0.218969	1.035163	2.284727
C	-1.372784	-2.857120	0.831553
C	4.212213	1.801101	0.230557
C	6.228778	-0.684324	-0.948646
H	2.090885	0.168753	1.392561
H	2.250180	-1.398823	2.191962
H	2.946143	-2.470203	0.213018
H	2.030926	-1.380292	-0.837206
H	0.158746	-0.815436	3.249794
H	-1.324859	-0.747059	2.292179
H	0.412519	-3.037253	1.987482
H	0.651706	-2.966096	0.238727
H	2.561217	0.903116	-0.694545
H	4.024645	0.850674	-1.656545
H	4.575442	-1.462397	-2.003334
H	5.029031	-2.368665	-0.559012
H	-0.785353	2.535348	3.447590
H	4.836415	3.674722	0.056689
H	8.042030	-0.973740	-1.697939
Hg	-2.497427	0.391975	-0.620321
O	-0.207224	0.018827	-1.090913

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H       0.057522 -0.443165 -0.154358
H      -0.111488 -0.596773 -1.842591
O      -2.946258 2.008559 1.094777
H      -2.292176 2.729430 1.168380
H      -3.142149 1.628873 1.972354
O      -3.294265 -0.979941 -2.472058
H      -4.028924 -0.579124 -2.973203
H      -3.541377 -1.865263 -2.144384
O      -4.539318 -0.853584 0.560660
H      -3.815225 -1.536681 0.563796
H      -5.204749 -1.045335 -0.125040
O      -3.365982 2.154063 -2.021960
H      -3.382612 3.032188 -1.598033
H      -3.027448 2.213390 -2.934410
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References

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