

Theoretical Prediction of Coordination Environments and Stability Constants of Lanthanum Lactate Complexes in Solution

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Supplementary Information

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[La(lac)(H₂O)₆]²⁺

Zero-point correction= 0.232565 (Hartree/Particle)
Thermal correction to Energy= 0.258477
Thermal correction to Enthalpy= 0.259422
Thermal correction to Gibbs Free Energy= 0.177537
Sum of electronic and zero-point Energies= -1236.411111
Sum of electronic and thermal Energies= -1236.385198
Sum of electronic and thermal Enthalpies= -1236.384254
Sum of electronic and thermal Free Energies= -1236.458139

La,0,-0.6715662647,-0.0401832783,-0.004777338
O,0,-2.6885898195,0.3291864744,-1.6404745201
O,0,-0.1142030004,1.4769700316,-2.1002562424
O,0,-1.1228698624,2.3470696756,0.8492304049
O,0,-2.8467500782,-0.2325455479,1.4668573686
O,0,0.0659981838,-1.4373985762,2.0386332606
H,0,-1.9738281229,-2.7477627193,-1.3513409631
H,0,-0.2886944896,2.6678314642,1.2295265303
H,0,-1.7647856554,3.0624658887,0.9389583449
H,0,0.6043957887,1.2737326041,-2.7136952947
H,0,-0.1712973736,2.4419047416,-2.0931861436
H,0,-0.972990076,-3.291885967,-0.3192657289
O,0,-1.3503955865,-2.4719470446,-0.6658251472
H,0,-2.559157569,0.7509535477,-2.5009052251
H,0,-3.6447567666,0.2706000766,-1.5174400539
H,0,-3.4539881207,-0.9683607944,1.6181866451
H,0,-3.081496762,0.4266193642,2.133851643
H,0,-0.2914880774,-2.0378123238,2.7045030004
H,0,0.8867616487,-1.0831893849,2.4109822721
O,0,1.1889681388,0.8408212369,0.7847921751
O,0,1.4818955273,-0.9267955574,-1.0309738972
C,0,2.456665421,0.785386825,0.3905297344
O,0,3.3420925408,1.4903578126,0.7877671739
C,0,2.7497026991,-0.2896081053,-0.654285644
H,0,3.1463541102,0.2202812811,-1.5472015283
C,0,3.7380700593,-1.3067380476,-0.142456629
H,0,3.9995318393,-2.0409328392,-0.9176523523
H,0,4.658108522,-0.7874197715,0.1533977181
H,0,3.3420463591,-1.8370192209,0.7362877304
H,0,1.6835373359,-1.7251815847,-1.5359996317

[La(lac)(H₂O)₇]²⁺

Zero-point correction= 0.257878 (Hartree/Particle)
Thermal correction to Energy= 0.285710
Thermal correction to Enthalpy= 0.286654
Thermal correction to Gibbs Free Energy= 0.202767
Sum of electronic and zero-point Energies= -1312.827536
Sum of electronic and thermal Energies= -1312.799705
Sum of electronic and thermal Enthalpies= -1312.798760
Sum of electronic and thermal Free Energies= -1312.882647

La,0,-0.5941293172,0.094026591,0.0289962811
O,0,-1.6335307833,-1.5821657457,-1.707907735
O,0,-0.0003439566,1.0380767522,-2.3196171348
O,0,-2.6922000411,1.3940983767,-0.9647380142
O,0,-2.8572277382,-0.5923322489,1.2017266758
O,0,-0.1276227372,0.1313000255,2.6683275277
O,0,-0.5984442616,2.6324207488,0.6399893421
H,0,-2.8004530637,2.3531992676,-0.9604864333
H,0,-3.3837562204,1.0568935576,-1.5478504683
H,0,0.8847435484,0.8592940624,-2.664206718
H,0,-0.3241704204,1.8070636875,-2.8045973406
H,0,0.3532995189,2.7696358386,0.7856905216
H,0,-1.0478797694,3.3940396517,1.0247437634
H,0,-1.4427610923,-1.5571783657,-2.6548470277
H,0,-2.2761380998,-2.2932925226,-1.5910682661
H,0,-2.967176863,-1.3388281534,1.8042343885
H,0,-3.6936654163,-0.1110085734,1.224223939
H,0,-0.5790862817,0.3420951785,3.4946873453
H,0,0.7451310873,0.5523310427,2.7153653948
O,0,1.4410198683,0.8812085248,0.5917132525
O,0,1.4741729995,-1.0524149965,-1.0833255827
C,0,2.6702433902,0.6449540321,0.1550205372
O,0,3.6337650576,1.3243200157,0.3845444765
C,0,2.8109360347,-0.6360185729,-0.6589793294
H,0,3.4025028247,-0.4050749943,-1.5582489449
C,0,3.4771038504,-1.7121897153,0.1632617208
H,0,3.594050777,-2.6417928913,-0.4117993604
H,0,4.477819352,-1.3730973636,0.4596868388
H,0,2.8966329597,-1.9198214195,1.0755928179
H,0,1.5481711156,-1.9216579245,-1.4966674746
O,0,-0.4004494291,-2.2211869046,1.2391041004
H,0,-0.0581843693,-2.0987030669,2.1370401661
H,0,-0.202371714,-3.1333204704,0.9940780828

[La(lac)₂(H₂O)₄]⁺

Zero-point correction= 0.267050 (Hartree/Particle)
Thermal correction to Energy= 0.294506
Thermal correction to Enthalpy= 0.295450
Thermal correction to Gibbs Free Energy= 0.208416
Sum of electronic and zero-point Energies= -1426.778359
Sum of electronic and thermal Energies= -1426.750902
Sum of electronic and thermal Enthalpies= -1426.749958
Sum of electronic and thermal Free Energies= -1426.836992

O,0,-0.2787840834,-1.2908681389,2.4378902922
O,0,-2.1148835146,-2.0721786983,-0.502366773
O,0,-3.9030485183,-0.1507966386,0.2906153493
O,0,-1.9002275852,0.3702053078,1.1458081697
O,0,-1.3986879757,1.3078889344,-1.2366188591
C,0,-2.9098612958,0.5652479514,0.3625265513
C,0,-2.6824879769,1.6855760674,-0.6531702836
C,0,-2.628369379,3.0641069218,-0.0528057605
H,0,-3.6059295922,3.3240451946,0.3753513925
H,0,-1.8757400497,3.1067999521,0.7457432216
H,0,-2.3894757003,3.8173230451,-0.8169330209
H,0,-1.2078842008,1.8702218054,-1.9957914855
H,0,-3.4546864614,1.6021212788,-1.4310794494
O,0,4.3649317659,0.1507138332,-0.1711194172
O,0,2.2566047674,-0.6180437601,-0.2569114498
O,0,1.2251101424,1.4215848281,0.8517839999
C,0,3.1831265665,0.2528940172,0.0622913585
C,0,2.6759281719,1.4902636403,0.8052577925
C,0,3.1385327061,2.7708573432,0.1561082419
H,0,4.2341225072,2.7780054378,0.1196924839
H,0,2.7566808617,2.8457966394,-0.8719992641
H,0,2.8063755513,3.6502183908,0.7264899324
H,0,0.8762867898,2.2104087884,1.2832826235
H,0,3.0540450052,1.4214994175,1.8388354106
La,0,-0.0529916986,-0.595918532,-0.0131807625
H,0,0.0816660915,-1.7843585591,3.1806806307
H,0,-1.1138528518,-0.8796761692,2.7123199055
H,0,0.9729563467,-3.8974506266,0.1500828085
H,0,-2.9506150103,-1.6649819081,-0.1721214039
O,0,1.0287901308,-2.9559658557,-0.0385438309
H,0,1.966572783,-2.7173868482,-0.1270934869
H,0,-2.3477744208,-2.9153937885,-0.9022230996
O,0,0.579604504,-0.8416888177,-2.5208835881
H,0,1.5411671631,-0.9302615333,-2.5841669434
H,0,0.2158543513,-1.0195478655,-3.3944206137

[La(lac)₂(H₂O)₅]⁺

Zero-point correction= 0.292491 (Hartree/Particle)
Thermal correction to Energy= 0.322421
Thermal correction to Enthalpy= 0.323366
Thermal correction to Gibbs Free Energy= 0.232677
Sum of electronic and zero-point Energies= -1503.187549
Sum of electronic and thermal Energies= -1503.157619
Sum of electronic and thermal Enthalpies= -1503.156675
Sum of electronic and thermal Free Energies= -1503.247363

O,0,0.6381528221,-2.1031448919,0.6244449955
O,0,-1.5855222939,-2.9391575351,-1.5895971377
O,0,-1.8968331335,0.9025376332,1.4877808704
O,0,-1.712648174,-0.8767258763,0.1428181402
O,0,-2.1010193399,0.70794264,-1.8589365349
C,0,-2.1494258248,0.3042022463,0.4523510414
C,0,-2.9191330961,0.9841084516,-0.6855581301
C,0,-3.1099195584,2.4622388239,-0.4933432127
H,0,-3.7026460063,2.643934951,0.4112391164
H,0,-2.1406508769,2.9642450716,-0.3690851218
H,0,-3.6444032106,2.9069408145,-1.3454804116
H,0,-2.4306060407,1.2264785542,-2.6009699186
H,0,-3.8851042747,0.4666083362,-0.8145662105
O,0,4.0500354159,0.4786799989,-0.1227386492
O,0,2.2895886698,-0.1808123079,-1.349790527
O,0,0.5613439517,1.0601644116,0.0974403519
C,0,2.8662895361,0.4819853032,-0.3731867379
C,0,1.9264218579,1.3286156293,0.485638025
C,0,2.2475782558,2.7990925108,0.3529034371
H,0,3.2944068078,2.9694439293,0.6316473556
H,0,2.1009565294,3.1298326696,-0.6860628318
H,0,1.6041515915,3.4020189437,1.0071189308
H,0,-0.0537957676,1.2790718058,0.8223845352
H,0,2.063410353,0.9996155128,1.5287211355
La,0,0.0203683341,-0.8171799715,-1.5463502076
H,0,1.4132936404,-2.3641568537,1.1317255377
H,0,-0.0626600151,-1.8443922607,1.2431917484
H,0,2.0904725959,-3.3172539835,-2.8119828363
H,0,-2.1207448633,-2.6197949215,-0.842119866
O,0,1.7978239457,-2.4780653741,-2.4459168425
H,0,2.5821774022,-1.9596287531,-2.1849032863
H,0,-1.4851987845,-3.8892712185,-1.471214607
O,0,0.8941690078,0.8517054369,-3.3790178307
H,0,1.7919422982,0.9147938381,-3.0087765812
H,0,0.7413263945,1.6423684073,-3.9053493014
O,0,-0.8973145433,-1.4088661983,-3.9257406906
H,0,-1.5520759766,-2.1043515243,-4.0545144451
H,0,-0.4923186393,-1.2331442892,-4.7816413227

[La(lac)₃(H₂O)₂]

Zero-point correction= 0.301188 (Hartree/Particle)
Thermal correction to Energy= 0.329697
Thermal correction to Enthalpy= 0.330641
Thermal correction to Gibbs Free Energy= 0.238718
Sum of electronic and zero-point Energies= -1617.019091
Sum of electronic and thermal Energies= -1616.990582
Sum of electronic and thermal Enthalpies= -1616.989638
Sum of electronic and thermal Free Energies= -1617.081561

O,0,-0.146334754,-0.0832080579,2.8089220632
H,0,1.4483657651,-4.0414912971,1.4321289383
O,0,-4.0484872059,1.6686782556,1.258421166
O,0,-1.9136907344,0.9585504118,1.2051795958
O,0,-2.2832491876,-0.3259121536,-1.1026285549
C,0,-3.102695737,1.1337251905,0.7104611365
C,0,-3.2587728378,0.6687473923,-0.7445685479
C,0,-3.032121888,1.8488759061,-1.6620775292
H,0,-3.7240063432,2.6606821423,-1.4062240814
H,0,-2.000221469,2.2213350834,-1.5444964607
H,0,-3.1793878887,1.5637510332,-2.7116631407
H,0,-2.5261450956,-1.2054056444,-0.7710545909
H,0,-4.2713183355,0.2592455281,-0.8750140895
O,0,3.9844312134,1.9112140603,-0.4868973074
O,0,2.2364468009,0.5158441577,-0.2857562132
O,0,0.6343585218,2.3233028883,0.5576262714
C,0,2.8333693827,1.6608588004,-0.1758555191
C,0,1.9869977468,2.7986762403,0.4127406648
C,0,2.036615665,4.0404542685,-0.4448429331
H,0,3.0788663704,4.3602002734,-0.5598131198
H,0,1.6221297192,3.8323336419,-1.441963966
H,0,1.4631022331,4.8609065,0.0110438225
H,0,0.0759391351,2.9846790059,0.9822098131
H,0,2.394550597,3.0084960586,1.4169290501
La,0,-0.0277560204,-0.1543400978,0.2124685192
C,0,-0.2873475398,-3.4956858213,0.296077641
H,0,-1.0220555846,0.3485940028,2.8282686877
O,0,-0.8027283008,-4.5973087748,0.261904694
O,0,-0.8687065815,-2.3530760926,0.1053837193
O,0,0.6596114009,-0.2270079689,-2.286876239
O,0,1.5877759325,-2.059293787,0.8313024219
H,0,0.4339081257,-0.5442951497,-3.1650499901
C,0,1.2257134651,-3.4248660609,0.5472392338
C,0,1.9727990096,-3.9373566385,-0.6628237161
H,0,1.6669361484,-4.9701281194,-0.8692987675
H,0,1.7378262069,-3.3191170355,-1.5432897108
H,0,3.0607396153,-3.9217424034,-0.4992470171
H,0,-0.0957441617,-0.7054417336,3.5389407136
H,0,2.5116486559,-1.8859575963,0.6088697499
H,0,1.6092542159,-0.0336305816,-2.2433376682

[La(lac)₃(H₂O)₃]

Zero-point correction= 0.329012 (Hartree/Particle)
Thermal correction to Energy= 0.359892
Thermal correction to Enthalpy= 0.360836
Thermal correction to Gibbs Free Energy= 0.266416
Sum of electronic and zero-point Energies= -1693.428414
Sum of electronic and thermal Energies= -1693.397533
Sum of electronic and thermal Enthalpies= -1693.396589
Sum of electronic and thermal Free Energies= -1693.491010

O,0,-0.1857912888,-0.049399679,2.824533638
H,0,1.5429870898,-3.8227545083,1.720526629
O,0,-3.7763501856,2.0971453526,1.1374102185
O,0,-1.7106133648,1.2167674681,1.0630599933
O,0,-2.3029248873,-0.4465640145,-0.9046326619
C,0,-2.9425469319,1.343773458,0.6678727369
C,0,-3.3525556159,0.4544197533,-0.5172695815
C,0,-3.7183232996,1.2969641205,-1.7178087412
H,0,-4.4661071216,2.0451269544,-1.4297027698
H,0,-2.8248635186,1.8119641781,-2.1016185048
H,0,-4.1226800698,0.6695224931,-2.5226486675
H,0,-2.3811431033,-1.2950155494,-0.4342923383
H,0,-4.2268777746,-0.1302416939,-0.1895069676
O,0,2.5601684786,2.647583604,-1.6239916626
O,0,2.256861143,0.5275852912,-0.96764348
O,0,1.8099598244,1.458222969,1.407209804
C,0,2.5827986233,1.7525081497,-0.7778857792
C,0,2.8948770301,2.0854176435,0.6910070922
C,0,2.9619736555,3.5591709062,0.9838206961
H,0,3.7591612921,4.0223448144,0.3895947518
H,0,2.013554473,4.044862391,0.716069195
H,0,3.1697982608,3.7408195496,2.0488703017
H,0,1.844657858,1.6544803561,2.3497598689
H,0,3.837090261,1.579538541,0.9677890233
La,0,0.0844058907,-0.062021647,0.1435911368
C,0,-0.3390791938,-3.3401693025,0.8224520925
H,0,-0.9810121129,0.5070106284,2.7074956295
O,0,-0.9104420272,-4.3837430079,1.0816231271
O,0,-0.8864597429,-2.1986644875,0.5509155906
O,0,0.5005269496,-0.9405703011,-2.2987276254
O,0,1.68443233,-2.0093014631,0.7204786131
H,0,-0.1218666039,-0.7646749998,-3.0108741547
C,0,1.1944027582,-3.3651006279,0.7807505108
C,0,1.6694847446,-4.1649258826,-0.4107588361
H,0,1.2635747522,-5.1817880848,-0.3475947205
H,0,1.3196129567,-3.7000357469,-1.3440525318
H,0,2.7679130009,-4.2312514071,-0.4345971724
H,0,-0.4912536868,-0.8661299312,3.2328558068
H,0,2.5864020693,-1.9910341082,0.380368564
H,0,1.2814274692,-0.3711719472,-2.4311813792
O,0,-0.1901468096,2.1126215059,-1.3777797363
H,0,0.6306692164,2.5172567032,-1.7244050613
H,0,-0.7327671025,2.8247473187,-1.0226379614