

Determination of thermodynamic functions and structural parameters of NpO_2^+ lactate complexes

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Supporting Information

Figures:

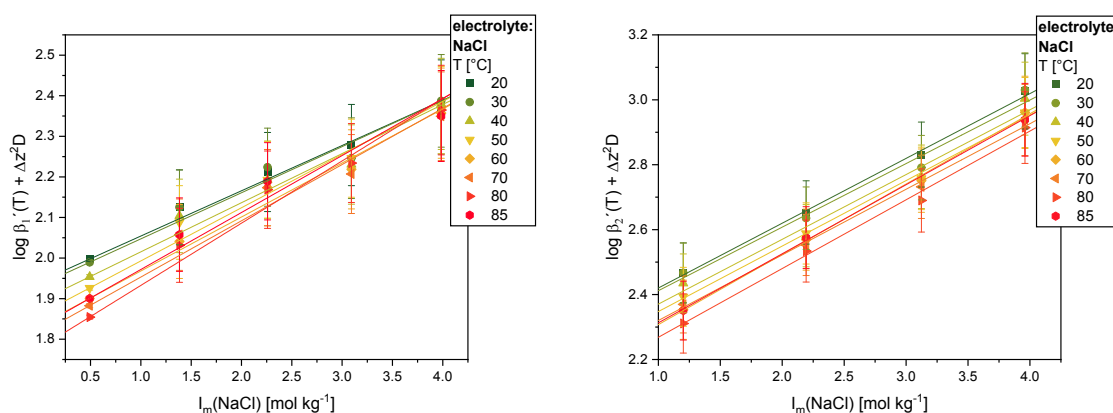


Figure S1: Ionic strength dependence of $\log \beta'_n(T) - \Delta z^2 D$ and linear fitting of the data according to the SIT for the complexation reaction $\text{NpO}_2^+ + n \text{Lac}^- \rightleftharpoons \text{NpO}_2(\text{Lac})_n^{1-n}$ ($n = 1, 2$) in NaCl.

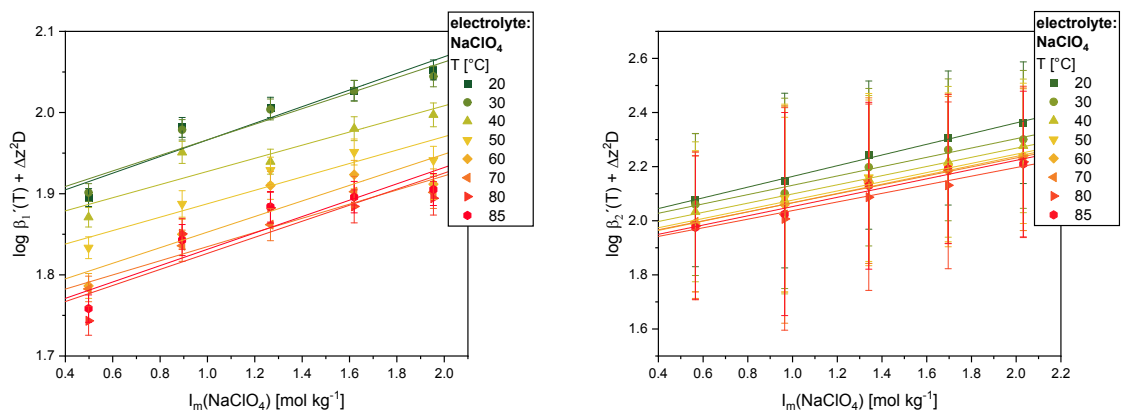


Figure S2: Ionic strength dependence of $\log \beta'_n(T) - \Delta z^2 D$ and linear fitting of the data according to the SIT for the complexation reaction $\text{NpO}_2^+ + n \text{Lac}^- \rightleftharpoons \text{NpO}_2(\text{Lac})_{n-1-n}$ ($n = 1, 2$) in NaClO_4 .

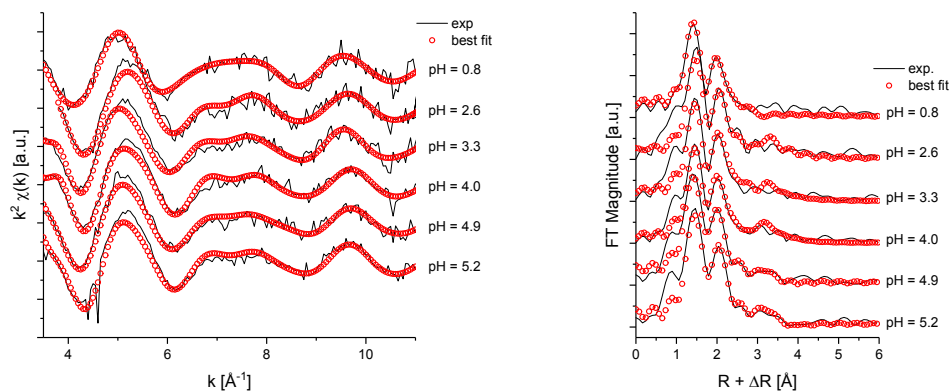


Figure S3: Raw k^2 -weighted Np-L₃-edge EXAFS spectra (left) and related Fourier transforms (right) of NpO_2^+ in the presence of lactate as a function of the pH_c value (black) and the corresponding fit curves (red circles).

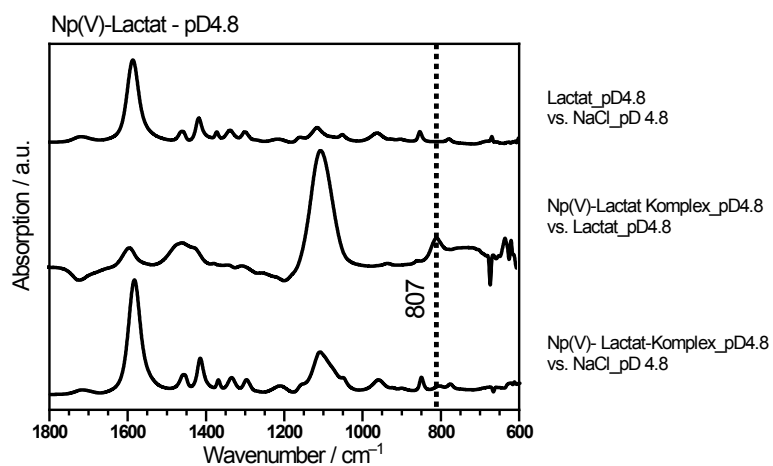


Figure S4: ATR-FT infrared spectra of lactic acid as a function of the pD_c value. $I_m(\text{NaCl}) = 1.0$, $T = 20^\circ\text{C}$, $[\text{Lac}^-]_{\text{total}} = 0.1 \text{ mol kg}^{-1}$.

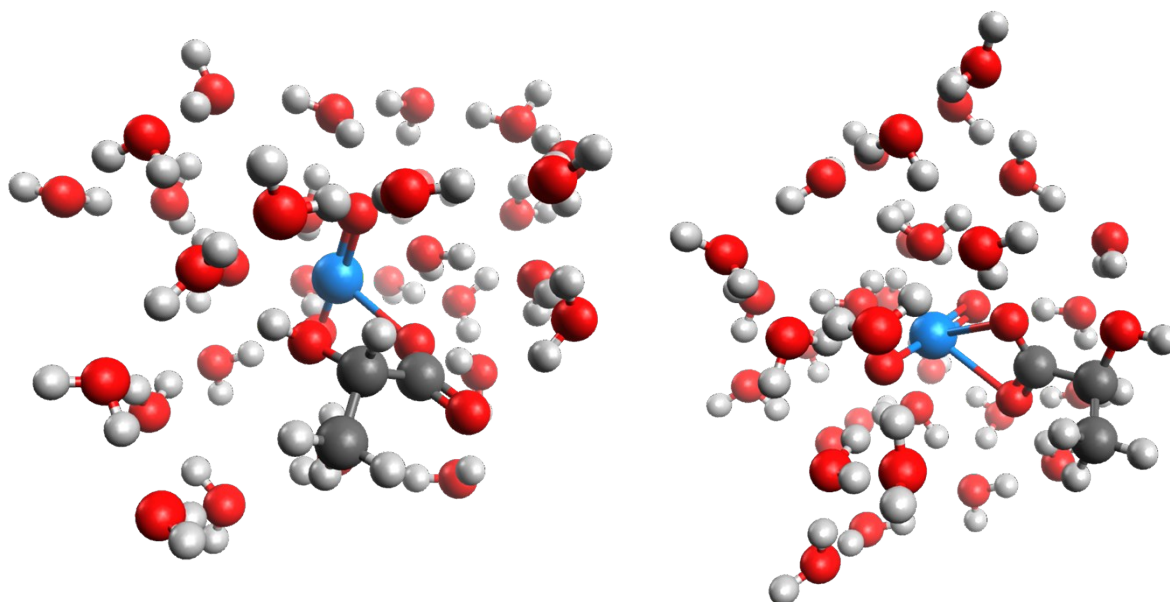


Figure S5: Structures of the optimized conformers of the $\text{NpO}_2(\text{Lac})$ complex with second hydration shell. (left) side-on coordination mode of lactate; (right) end-on coordination mode of lactate.

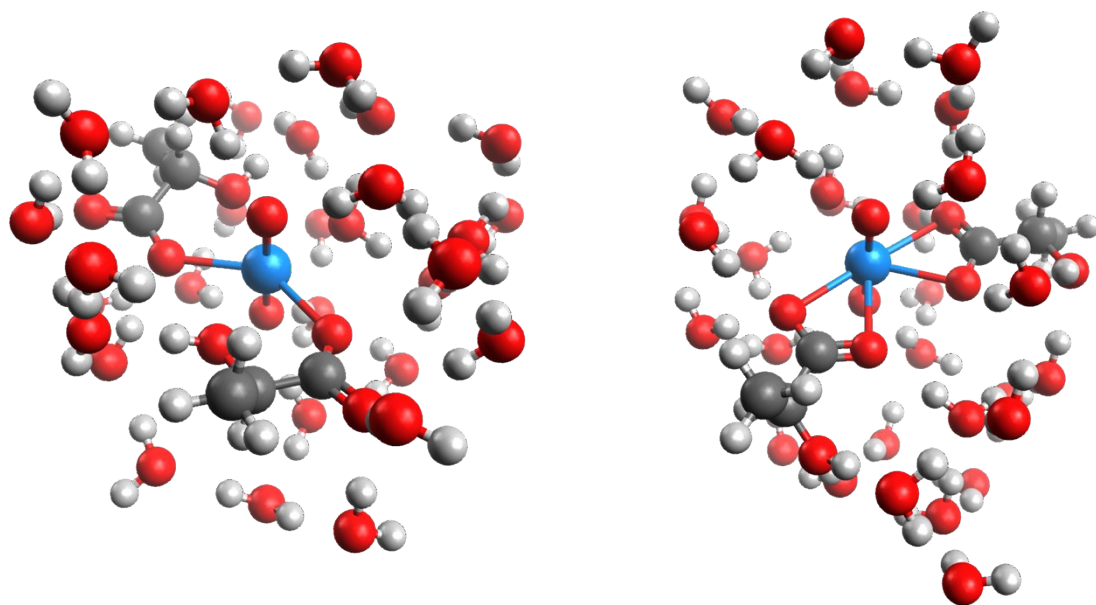


Figure S6: Structures of the optimized conformers of the $\text{NpO}_2(\text{Lac})_2^-$ complex with second hydration shell. (left) side-on coordination mode of lactate; (right) end-on coordination mode of lactate.

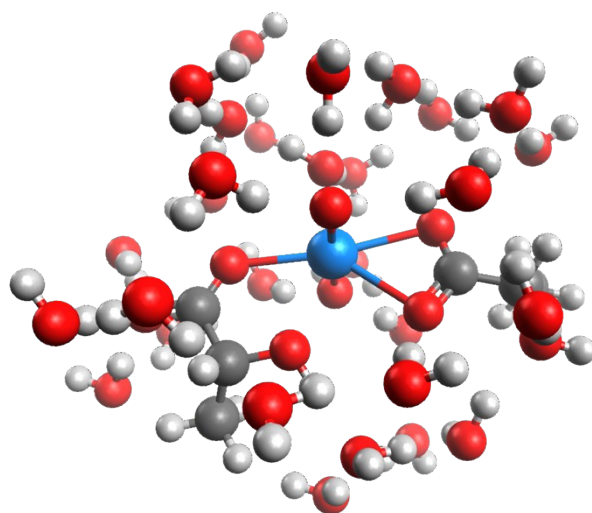


Figure S7: Structure of the optimized conformer of the $\text{NpO}_2(\text{Lac})_2^-$ complex with one end-on and one side-on coordinating lactate and second hydration shell.

Tables:

Table S1: Fit parameters of the raw k^2 -weighted Np-L₃-edge EXAFS spectra shown in Fig. S1. * fixed for fitting.

pH		5.2	4.7	4.0	3.3	2.6	0.8
k-weighting		2	2	2	2	2	2
O _{ax}	N	2*	2*	2*	2*	2*	2*
	R / Å	1.84 (1)	1.84 (1)	1.84 (1)	1.83 (1)	1.85 (1)	1.83 (1)
	$\sigma^2 / \text{Å}^2$	0.00028 (30)	0.00042 (23)	0.00034 (36)	0.00038 (29)	0.00051 (38)	0.00066 (60)
O _{eq}	N	4.1 (1)	4.2 (1)	4.1 (1)	4.2 (1)	3.1 (1)	4.9 (1)
	R / Å	2.48 (1)	2.48 (1)	2.49 (1)	2.49 (1)	2.51 (2)	2.48 (1)
	$\sigma^2 / \text{Å}^2$	0.0067 (14)	0.0074 (14)	0.0056 (10)	0.0067 (17)	0.0026 (22)	0.0062 (21)
C _c	N	2.5 (1)	1.3 (1)	1.2 (1)	1.1 (1)	1.3 (1)	-
	R / Å	3.23 (2)	3.14 (2)	3.12 (4)	2.81 (4)	2.72 (8)	-
	$\sigma^2 / \text{Å}^2$	0.004*	0.004*	0.004*	0.004*	0.004*	-
molar fractions [%]	⁻ NpO ₂ ⁺	0	0	0	0	24	100
	NpO ₂ (Lac)	47	52	66	72	68	0
	NpO ₂ (Lac) ₂	53	48	34	28	8	0
S ₀ ²		0.9	0.9	0.9	0.9	0.9	0.9
$\Delta E_0 / \text{eV}$		12.7 (5)	11.9 (4)	11.4 (6)	11.6 (5)	14.1 (5)	10.6 (8)
Red error		0.015083	0.0107628	0.0254695	0.0151136	0.0204184	0.0486686

Table S2: Species distribution of the NpO₂(Lac)_n¹⁻ⁿ complexes (n = 0 – 2) in the EXAFS samples as a function of the pH_c value.

pH	NpO ₂ (H ₂ O) ₅ ⁺	NpO ₂ (Lac)	NpO ₂ (Lac) ₂ ⁻
0.8	1.00	0.00	0.00
2.6	0.24	0.68	0.08
3.3	0.00	0.72	0.28
4.0	0.00	0.66	0.34
4.7	0.00	0.56	0.44
4.9	0.00	0.52	0.48
5.2	0.00	0.47	0.53

Structural data of the DFT calculations

xyz data:

Complex species: NpO₂(Lac) with end-on
coordinating ligand

C	0.4372701	0.7410249	-5.5807065	H	4.8342992	-1.8104270	-1.7327562
C	-0.7757944	0.9755630	-4.6996527	H	-2.4576621	-4.3279958	0.1000108
O	-1.2597174	2.3023949	-4.7988973	H	5.9459341	-2.8844197	-1.6339892
C	-0.4363311	0.7057788	-3.2509754	H	-1.5369876	-4.4657290	-1.1333538
O	-0.3530324	1.6419802	-2.4358401	H	2.2707513	-4.2348409	-1.5798348
Np	0.0376473	0.1809816	-0.4272225	H	-4.4391146	-3.4572044	-3.0860595
O	-0.3628443	2.4794886	0.2744412	H	3.7373106	-3.8759185	-1.2594103
O	-0.2359972	-0.4778123	-2.9000350	H	-3.3442710	-3.4634463	-1.9960812
O	0.2899396	-0.1138148	1.9634408	H	-0.2544308	-3.8644109	-2.9397303
O	1.8258573	0.4791529	-0.5805514	H	-0.7974156	-1.9720891	-3.6711297
O	0.4463948	-2.2774498	-0.2550555	H	0.3651559	-5.2313534	-2.4790973
O	-1.7289976	-0.0822260	-0.1920266	H	-2.0321674	-2.8910221	-3.7232995
O	-2.3075453	0.2031079	2.6960055	H	4.4113809	0.3903960	-2.4523052
O	2.2388327	0.2712539	3.6679359	H	3.4383159	-0.1027767	-1.3671275
O	0.6697760	3.6531618	2.4949097	H	0.3690120	-2.9583116	-0.9273795
O	-2.6743720	3.6721300	-0.5440841	H	0.9532863	-2.6685636	0.4724618
O	-3.5124722	2.5918487	-2.8815449	H	-2.3471758	-1.5359681	3.4233842
O	-1.0913071	-2.8586048	-3.9255878	H	2.4599500	-4.0907074	0.6579827
O	0.1723874	-4.3457522	-2.1886202	H	-1.3659217	-2.5618697	4.0723152
O	3.3521460	2.6982578	2.7629402	H	1.4150650	-4.4656122	1.7752551
O	2.9180466	-2.4214985	3.6308892	H	-3.2151613	-4.9421611	2.2641555
O	2.0011626	-3.7689443	1.4577436	H	3.6637586	-2.8826918	3.9997980
O	2.9797283	-4.4046255	-0.9620779	H	-2.4079585	-3.6495378	2.5406435
O	4.3647854	-0.1246978	-1.6329345	H	2.7003462	-2.8640289	2.7918366
O	5.0119739	-2.7662137	-1.7595306	H	0.0751918	-6.3445836	2.7705438
O	-1.7875392	2.8476962	3.6651822	H	0.3087903	-4.0802982	4.0824572
O	-3.2464910	4.3799587	2.0850254	H	-0.8499841	-5.1737038	2.3534702
O	-2.1415648	6.3146597	0.3493807	H	1.1088341	-2.8355396	4.4546126
O	-3.5846722	-0.1148900	-2.3322167	H	-2.2762791	1.1079195	3.0296438
O	0.0561733	-5.4048514	2.6232943	H	-2.4837887	0.2370784	1.7519237
O	-2.4367887	-4.4690140	1.9859649	H	-1.1806078	2.9290014	-0.0106036
O	-2.2258925	-2.4638576	3.6417134	H	-0.0131922	2.8948160	1.0748365
O	0.2622385	-3.2659264	4.5857339	H	3.9798463	3.2960807	3.1553623
O	0.6707482	4.1981570	-2.2963644	H	-3.3692135	3.8896546	1.2661372
O	0.4165976	5.6059303	0.2387380	H	3.6228169	2.5632137	1.8368056
O	3.8075613	2.1858488	0.1406167	H	-2.9444746	5.2359757	1.7671290
O	-2.4543983	-4.4256538	-0.8582402	H	2.9940976	1.6990396	-0.0734665
O	-3.6804721	-2.9766077	-2.7721414	H	-2.0305882	2.9810000	4.5759896
O	3.4942901	3.7508533	-2.2891396	H	4.4882058	1.5924285	-0.1825657
O	4.3107870	1.6349941	-3.7634595	H	-2.3289018	3.4751057	3.1363152
H	-3.7302249	1.6588041	-2.7564139	H	-1.1745355	6.1636776	0.3109228
H	2.5572382	3.9692398	-2.3276792	H	1.5387947	3.3204026	2.7460383
H	-2.7711984	2.5906835	-3.4890666	H	-2.2877601	7.2403571	0.1831015
H	3.6537637	3.4511628	-1.3915143	H	0.0049938	3.3242858	3.1108339
H	-2.6234812	4.6249340	-0.6374834	H	2.7115749	-0.5663562	3.7041769
H	5.0046933	1.8721816	-4.3672854	H	2.8427013	0.9908035	3.4717396
H	-3.0236763	3.2952766	-1.3748423	H	1.0259962	0.0605513	2.5888358
H	4.0185078	2.4560461	-3.3292585	H	-0.5486130	-0.0916615	2.4434848
H	0.5630804	5.0699092	-0.5473677	H	-1.4901601	2.4756139	-5.7064495
H	0.2669078	3.3176751	-2.3444399	H	-1.5647711	0.2751534	-4.9612916
H	0.6266249	5.0633028	1.0016223	H	0.1869713	0.9334339	-6.6193505
H	0.3180731	4.6766761	-3.0392883	H	1.2548695	1.3912639	-5.2922500
H	-3.7805972	-1.0280027	-2.5497516	H	0.7659914	-0.2871501	-5.4995230
H	-3.0294386	-0.1481582	-1.5474110				

Complex species: NpO₂(Lac) with side-on
coordinating ligand

C 0.2618919 -0.8286896 -2.9810659
C -0.2378842 0.6006786 -3.1535032
O 0.0199073 1.3044732 -1.9395131
Np 0.1395017 0.0116128 0.2322971
O 0.0643102 0.1057081 2.6885583
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O 0.4677848 -1.2112487 -1.7926999
O 1.9623355 0.1491497 0.4054360
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O 0.0139076 -2.3956934 0.8130408
O 0.0065773 2.4535726 0.7034042
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H -2.8693416 3.0254535 2.6119262
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H 0.8366878 -0.1894069 3.1878903
H -0.7772116 -0.1559856 3.0856198
H 0.2451652 6.3162405 -2.1870493
H -1.3144746 0.5200651 -3.2863522
C 0.3847391 1.2989633 -4.3380311
H 0.2087416 0.7173253 -5.2326671
H -0.0558782 2.2820935 -4.4625231
H 1.4528295 1.4075234 -4.1936373

Complex species: $\text{NpO}_2(\text{Lac})_2^-$ with two end-on
coordinating ligands

C 1.9401480 -4.2386944 -2.1050476
C 1.0663696 -3.1553203 -2.7039334
C 0.4639055 -2.2806093 -1.6158640
O -0.2479032 -2.8194972 -0.7265767
Np -0.9449387 -0.4537782 0.1667347
O -1.5939403 1.9001143 0.8384890
O 1.8304766 -2.4276810 -3.6209390
O 0.6413748 -1.0501597 -1.6296517
O 0.3247366 -0.5304051 1.4490001
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O 0.2981978 -0.1842756 -4.3246984
O 2.8117775 3.6211801 1.4971561
O 0.3370779 1.0918112 4.0339043
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O -2.3657603 -0.7681591 -3.9028907
O 0.3566947 -4.2691211 1.7973222
O 2.8686407 -3.6333531 2.7538131
O 3.7960200 -0.6255880 -2.6010737
O 2.6096066 1.7016648 -1.9380505
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O -3.9433536 -3.1414866 -3.5276475
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O -5.6229602 -1.2816150 2.2400968
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H -1.6480931 -3.9610340 -1.2739169
H -4.5471735 -4.2999896 0.9217338
H -2.8189508 -4.0466652 -2.2889466
H 3.6447439 -1.1582539 0.9407720
H 2.1768931 -0.9046665 1.4639543
H -3.1841049 -2.3591420 1.1025888
H -2.1951597 -2.2930353 2.3008348
H -3.5243174 2.1802148 0.9980870
H -0.7145404 -3.7000031 2.9312356
H -4.3107545 1.5994929 2.1543663
H -1.8427321 -4.0397329 3.9514081
H -4.0881932 -0.2825204 -0.6067772
H -0.9156726 -0.2256275 4.7678424
H -4.9684477 0.6968140 0.1585525
H -1.4432887 -1.6417848 4.4876310
H -6.5648249 -1.1596824 2.2905997
H -4.5325638 -0.1920011 3.3586075
H -5.3744729 -1.0273585 1.3401304
H -3.1980884 -0.0014776 4.1110169
H 2.1113101 5.1243675 -2.7964008
H 1.0925600 4.1458570 -3.3831285
H 1.7683358 2.3900214 4.3065490
H 4.3219458 4.7553585 -3.5807300
H 3.2681495 2.4376128 4.0832387
H 4.2878875 4.6418264 -2.0590351
H 3.6400796 2.0105428 1.9945414
H -2.7021918 2.1597967 3.8311906
H 3.7932504 0.5266933 2.3806679
H -1.8850237 2.4927880 2.5937172
H 3.8102881 2.7352390 -1.1630718
H 2.5938741 3.7438792 2.4280445
H 4.0938042 3.6061852 0.0670568
H 2.0525093 3.9000881 0.9648448
H -0.4213093 1.6874212 3.9157372
H 0.4483787 0.6414708 3.1935943
H 1.2919766 -1.7454943 -4.0469489
H 0.2176142 -3.6234038 -3.2035507
H 2.3251578 -4.8652482 -2.8993136
H 2.7809360 -3.7983477 -1.5803706
H 1.3775530 -4.8494148 -1.4118862
C -0.7050081 2.4362026 0.1105622
C -0.5656282 3.9465977 0.1537034
O 0.7288577 4.3590584 -0.1508717
C -1.6135830 4.5834553 -0.7466818
H -0.7611446 4.2362310 1.1814253
H 0.8577230 4.4914000 -1.1129316
H -1.5388138 5.6610177 -0.6705252
H -1.4490151 4.3050032 -1.7809525
H -2.6113691 4.2807188 -0.4518024

Complex species: $\text{NpO}_2(\text{Lac})_2^-$ with two side-on
coordinating ligands

C 2.2046226 -2.6466012 -3.6299923
C 1.3651267 -1.5643699 -2.9926975
O 1.7361709 -1.3283387 -1.6426064
Np 0.0187592 -0.2864540 -0.0955737
O 0.1672656 1.2083055 -1.1036509
C -0.1227552 -1.8958606 -3.0010991
O -0.7870252 -1.5271939 -1.9931114
O -0.5908013 -2.4612264 -3.9856442
O -2.4656108 0.1146475 -0.2260379
C -3.1591028 0.9103272 0.7207377
C -2.1400167 1.4503953 1.7229875
O -2.5492772 2.2554906 2.5781910
O 2.2120681 0.1414994 0.9021058
O -0.9703040 1.0353269 1.6330892
O -0.0794969 -1.8173448 0.9238303
C -3.9409149 2.0196932 0.0507950
O 2.2588378 0.7391717 3.5138322
O 4.0474651 1.6573499 -0.3522441
O 2.8125664 3.3495259 -2.0641743
O 1.7760340 3.2045605 2.4831899
O 0.8246339 -1.2081268 4.7384865
O -0.4932114 4.3094968 3.5053665
O 4.5060733 3.2949481 2.0889079
O 4.8614053 1.3590690 4.1120247
O -1.3893505 -2.2756001 3.4972388
O -4.1018595 -1.7910658 3.4101611
O -3.8843176 -0.2197017 -2.5883040
O -2.5475225 -0.6917422 -4.8557054
O 0.9568145 1.8907452 -3.6701652
O -3.5816031 4.7617586 1.9234699
O -3.8236069 2.4158494 -3.5174177
O -1.6043706 2.0156037 -5.0876507
O -4.2679628 0.9152912 4.3204929
O -0.9883265 5.6900742 1.1232134
O 1.6393115 -3.0626194 2.5956456
O 3.9793528 -3.1025386 1.2971473
O 3.4113639 -4.7775547 -0.7710030
O 5.4301753 -3.5104053 -2.2163041
O 4.3938007 -1.2085481 -0.9566782
O 0.7682556 3.7823958 -0.0800431
O -4.8397131 -2.1229528 0.6906762
O -3.2951817 -2.8051220 -1.4910824
O -1.6756591 -4.8339010 -2.5287768
O 0.3818297 -4.3904938 -0.5613640
H 2.2817132 2.9706967 -2.7728552
H 3.1489152 -3.0750891 1.8131083
H 2.1762616 3.7288951 -1.4478810
H 4.6936954 -3.1157232 1.9252051
H 4.4750423 0.9144899 -0.7791701
H 3.3681123 -5.6961460 -0.5254481
H 3.6783978 2.2381515 -1.0475509
H 3.6562171 -4.2813653 0.0265721
H 4.8991628 -1.8778492 -1.4337654
H 5.4143667 -3.5959700 -3.1632375
H 2.6932375 -1.2134344 -1.5344221
H 4.7349544 -4.0870669 -1.8760142
H 0.1853274 2.0390693 -4.2203583
H 0.6084014 1.6127111 -2.8157065
H -0.9669330 -4.8160598 -1.8766719
H -3.7998463 3.0019388 -2.7680580
H -1.3866890 -4.2313107 -3.2169154

H -4.0815031 1.5540755 -3.1691023
H -2.4836368 -2.2981935 -1.6187105
H -1.7222880 2.4973694 -5.8992896
H -3.0272138 -3.6862230 -1.7806873
H -2.3592409 2.2484467 -4.5221810
H -3.3672624 -0.4281113 -3.3963606
H -1.9057741 -1.3938269 -4.6892438
H -4.2707066 -1.0580949 -2.3332633
H -2.0526234 0.0943018 -5.0972702
H 1.3193661 -4.3407723 -0.7448282
H 0.1499408 -3.5658995 -0.1255646
H -2.9500946 0.0425930 -1.0643536
H -0.4811179 5.1191577 0.5358566
H -4.2143360 -2.4104613 0.0068445
H -1.9087307 5.4247473 1.0703023
H -5.6430069 -2.6031299 0.5239050
H -4.2881519 -0.8833483 3.6697787
H -4.3969881 -1.9021219 2.5005677
H -3.6224720 5.2750198 2.7238136
H -3.3043871 3.8779808 2.1982743
H 1.1520687 3.5616147 0.7818477
H 0.4186691 2.9479774 -0.4091131
H 2.8264946 0.7745052 0.4838607
H 2.2704399 0.2745403 1.8684967
H -0.0857342 -1.4127954 4.4798033
H 4.5196333 2.8093436 1.2611331
H 1.3205899 -1.8884261 4.2839472
H 4.8365095 2.6867871 2.7567795
H 1.0358705 -2.5539367 2.0198737
H 1.1653236 3.7519408 2.9995311
H 1.1424109 -3.8405731 2.8355627
H 2.6852471 3.5324712 2.5027945
H 5.3983955 0.5855866 4.2334857
H 1.6228467 0.2134193 4.0285025
H 3.9446089 1.0542584 4.0297142
H 1.8875799 1.6126031 3.3058753
H -2.3504631 -2.1680357 3.5600396
H -1.1719375 -2.0830297 2.5837501
H 4.2331115 -1.5879913 -0.0882281
H 1.4654759 -0.6371506 -3.5548308
H 1.8389191 -2.8417787 -4.6287034
H 3.2397881 -2.3287801 -3.6885508
H 2.1520720 -3.5625350 -3.0533665
H -3.8409286 0.2711382 1.2746003
H -4.4942044 2.5891625 0.7832043
H -3.2689201 2.6959232 -0.4681499
H -4.6445000 1.5982452 -0.6574347
H -0.6683045 4.9075562 2.7652612
H -3.8544964 0.9186415 5.1774048
H -1.0549267 3.5463351 3.3471109
H -3.7051310 1.4670980 3.7615778

Complex species: $\text{NpO}_2(\text{Lac})_2^-$ with one end-on
and one side-on coordinating ligand

C -3.8752164 2.0163663 0.0423871
C -3.1577823 0.8795921 0.7380404
C -2.1169417 1.3825981 1.7376238
O -2.4954934 2.2074572 2.5869970
O -2.5083033 0.0273936 -0.1925602
Np -0.0391306 -0.4690369 -0.0533123
O 0.1837877 1.0027354 -1.0717760
O 1.3176951 -1.8062616 -1.6814775
O 2.2394556 -0.1700949 0.8502890
O -0.8171334 -1.6786731 -2.1172278
O -0.9653308 0.9193668 1.6507237
O -0.2239634 -1.9871709 0.9614806
O 2.2480033 0.4857924 3.4084870
O 4.0302517 1.3518885 -0.3591758
O 2.8488358 3.0606381 -2.1233621
O 1.8437602 2.9880501 2.4485333
O 0.7482018 -1.3694604 4.6850645
O -0.3676781 4.1946137 3.4968739
O 4.5526227 2.9844498 2.0401093
O 4.9478858 0.8594598 3.8813528
O -1.5741661 -2.3076241 3.5271649
O -4.2755844 -1.7271426 3.3308383
O -3.9211523 -0.2442482 -2.5584174
O -2.4485301 -0.7844531 -4.7216564
O 0.8974829 1.6631375 -3.6991792
O -3.4573440 4.7434656 1.9358693
O -3.9300800 2.3643190 -3.5273525
O -1.6847559 1.9341085 -5.0297082
O -4.3556628 0.9711299 4.2595521
O -0.8347876 5.5656601 1.1006607
O 1.4790749 -3.3892435 2.6804032
O 3.4726498 -2.6849197 0.8352326
O 2.9009989 -4.4639273 -1.0968559
O 4.3942719 -2.9601962 -2.9721463
O 5.2952350 -1.0919169 -0.9918673
O 0.8360405 3.5947801 -0.1048270
O -4.9760792 -2.0900443 0.5890971
O -3.4095457 -2.8746486 -1.5642618
O -1.9272374 -5.0012923 -2.5524401
O 0.0331618 -4.5932885 -0.5740115
H 2.2950336 2.6875904 -2.8166498
H 3.0365295 -3.0417304 1.6167237
H 2.2363214 3.4725992 -1.5054266
H 3.0514457 -1.8220848 0.7126628
H 4.5856363 0.6586886 -0.7369594
H 3.2960754 -5.2662448 -0.7704100
H 3.6936241 1.9159115 -1.0804655
H 3.0834350 -3.7812360 -0.4178508
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H 0.0938773 1.8956299 -4.1666082
H 0.6078693 1.3448029 -2.8381951
H -1.2539103 -4.9912095 -1.8596544

H -3.9343924 2.9722378 -2.7951844
H -1.5795879 -4.4304943 -3.2384083
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H 1.0436396 -4.1994995 2.9273017
H 2.7700212 3.2696084 2.4631498
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H 4.0036541 0.6482417 3.8569824
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H -0.9550070 3.4493017 3.3485360
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H 1.1054155 -0.8725539 -4.7611306
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