Supplementary Material (ESI) for Chemical Communications

The highest water exchange rate ever measured for a Gd(III) chelate

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Electronic Supplementary Information

***N,N´*-Bis(6-carboxy-2-pyridylmethyl)ethylenediamine-*N,N´*-methylenephosphonic acid (H_6L).** 1,2-[{6-(Methoxycarbonyl)pyridin-2-yl}methylamino]ethane (1.4 g, 3.91 mmol) and phosphorous acid (2.5 g, 30.5 mmol) were dissolved in 20 cm^3 of 6M aqueous HCl. The resulting mixture was heated under an inert atmosphere (Ar) for 30 min and paraformaldehyde (0,94 g, 30.5 mmol) was added in portions over a period of 48h. After the addition of paraformaldehyde was complete the reaction mixture was refluxed for 48 h. The resulting brown solution was concentrated under vacuum to obtain a brown oil that was dissolved in a ethanol : water mixture (1:1, 2 mL). Upon stirring this solution for 24 h at room temperature a white precipitate was formed, which was collected by filtration and dried under vacuum at 40 ºC. Yield: 0.89g (44 %). ^{1}H NMR (200 MHz, D_2O, 25 ºC, TMS, pD = 7.0): δ = 7.69 (d, 4H, py), 7.34 (t, 2H, py), 4.07 (s, 4H, -CH_2-), 3.00 (s, 4H, -CH_2-), 2.81 ppm (d, 4H, -CH_2-, J_{HP}=11Hz); ^{13}C NMR (50.4 MHz, D_2O, 25 ºC, TMS, pD = 7.0): δ = 52.1, 54.9, 60.4 (secondary C), 124.8, 127.3, 140.3, (tertiary C), 154.5, 173.8, (quaternary C); ^{31}P NMR (200 MHz, D_2O, 25 ºC, TMS, pD = 7.0): δ = 12.18 ppm; Elemental analyses calcd. (%) for $C_{18}H_{24}N_4O_{10}P_2 \cdot 2H_2O$: C 39.0, H 5.1, N 10.1. Found: C, 38.8; H, 4.8; N, 10.1. IR (KBr): 1738 (C=O), 1597 cm^{-1} (C=C py), 1358 cm^{-1} (P=O).

$[Lu(L)(H_2O)]^{3-}\cdot 19H_2O$ (vacuo) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	71	-0.242873	-0.107955	0.589800
2	7	-0.698277	2.419976	0.126061
3	7	0.608234	-2.660842	-0.128586
4	7	-1.154188	-1.648451	-2.161862
5	7	0.238788	1.055005	-2.240654
6	8	-2.328180	-0.018156	0.065798
7	8	1.800701	0.627397	0.170574
8	15	-3.397289	-0.638817	-0.988204
9	15	2.661183	0.724009	-1.097465
10	8	-3.823478	0.367584	-2.042484
11	8	-4.556574	-1.230437	-0.196068
12	8	3.941657	1.521730	-0.885182
13	8	2.938029	-0.646956	-1.708964
14	6	-0.873264	5.150372	-0.053466
15	6	0.773520	-4.723316	-1.286805
16	6	0.349772	-3.396625	-1.207898
17	6	-0.312908	-2.810080	-2.426263
18	6	-1.161820	-0.731696	-3.321993
19	6	-2.521174	-2.036233	-1.737477
20	6	1.784549	-4.496833	0.843401
21	6	1.323382	-3.204030	0.863821
22	6	1.627875	-2.361026	2.067065
23	6	1.495650	-5.279363	-0.259268
24	6	-0.860121	4.536962	1.180884
25	6	-0.752749	3.167382	1.219399
26	6	-0.644497	2.453422	2.526029
27	6	-0.811266	4.373022	-1.193314
28	6	-0.753064	2.995742	-1.072890
29	6	-0.798795	2.103747	-2.286177
30	6	0.104398	0.111873	-3.375121
31	6	1.621539	1.644905	-2.250754
32	1	-0.906403	6.218673	-0.133462
33	1	0.542138	-5.286306	-2.167009
34	1	0.500842	-2.544823	-3.089298
35	1	-0.886265	-3.596099	-2.921052
36	1	-1.231066	-1.302785	-4.251967
37	1	-2.047494	-0.125440	-3.257577
38	1	-2.444558	-2.806507	-0.985162
39	1	-3.087709	-2.463636	-2.566830
40	1	2.347036	-4.846412	1.679645
41	1	1.832775	-6.295517	-0.314927
42	1	-0.894066	5.073453	2.102974
43	1	-0.742669	4.821761	-2.158925
44	1	-1.772823	1.636894	-2.305105

45	1	-0.687337	2.716765	-3.180521
46	1	0.109314	0.670340	-4.315808
47	1	0.973362	-0.523207	-3.375526
48	1	1.575349	2.683678	-1.958713
49	1	2.039598	1.608582	-3.254645
50	8	1.158152	-1.192045	2.069867
51	8	2.301722	-2.881062	2.981652
52	8	-0.510597	1.169097	2.426209
53	8	-0.645120	3.095214	3.575386
54	8	3.861610	-0.038719	-4.266171
55	1	3.425679	-0.196249	-3.410858
56	1	4.777273	0.181985	-3.997529
57	8	5.939547	0.501933	-2.624094
58	1	5.366323	1.067754	-2.065468
59	1	5.985253	-0.349644	-2.152203
60	8	0.846047	0.073896	4.433695
61	1	1.386731	-0.357606	3.743685
62	8	-0.276077	-2.366594	4.413490
63	1	0.023567	-1.466066	4.669548
64	1	0.528812	-2.869302	4.214949
65	1	0.158378	0.528990	3.888980
66	8	1.881365	2.596582	4.653700
67	1	1.010710	3.004468	4.491318
68	1	1.697067	1.644783	4.784660
69	8	4.859626	-1.806898	2.097931
70	1	4.944047	-2.067984	1.164573
71	1	4.062013	-2.187009	2.497608
72	8	2.212503	2.746991	1.946629
73	1	2.276739	2.676074	2.921586
74	1	2.161095	1.883653	1.499564
75	8	5.715449	0.510076	0.952010
76	1	5.036502	1.036114	0.480483
77	1	5.310893	-0.060869	1.632896
78	8	3.167810	4.042472	-0.151647
79	1	2.761398	3.788681	0.710299
80	1	3.631570	3.238754	-0.465537
81	8	5.390824	-1.531249	-0.724124
82	1	5.667656	-0.763538	-0.166008
83	1	4.487404	-1.347759	-1.064118
84	8	2.486059	-2.405035	-3.757292
85	1	2.627592	-2.020748	-2.869755
86	1	2.972540	-1.810080	-4.353039
87	8	1.996649	5.053286	-2.259144
88	1	2.365252	4.764186	-1.376770
89	1	2.602398	4.699179	-2.925971
90	8	-1.519917	-1.598549	2.063103
91	8	-3.929645	-0.748429	2.397206
92	8	-5.026751	2.475280	-0.863188
93	8	-6.785562	0.275861	-0.259479
94	8	-2.189735	-4.042735	1.066242

95	8	-4.638125	-4.081534	-0.324637
96	8	-6.433149	1.168169	-2.786727
97	8	-3.670828	1.787760	1.479145
98	1	-3.946710	0.230427	2.343060
99	1	-4.271336	2.270754	0.885352
100	1	-3.068900	1.258053	0.920452
101	1	-6.292411	1.091186	-0.071926
102	1	-6.106882	-0.439223	-0.220877
103	1	-4.384329	1.832830	-1.243766
104	1	-5.736801	2.479355	-1.531098
105	1	-5.523310	0.814256	-2.840134
106	1	-6.812979	0.733631	-1.992718
107	1	-4.807856	-3.123028	-0.303420
108	1	-3.847222	-4.221753	0.225450
109	1	-2.450702	-1.228869	2.239500
110	1	-1.092431	-1.871241	2.908825
111	1	-1.974666	-3.153755	1.425052
112	1	-1.393063	-4.423720	0.683490
113	1	-4.311879	-1.067781	1.548567

HF=-3880.0804769 Hartree
Zero-point correction= 0.966038 Hartree
Sum of electronic and thermal Enthalpies= -3879.042376
Sum of electronic and thermal Free Energies= -3879.217658

$[Lu(L)]^{3-}\cdot 20H_2O$ (vacuo) (0 imaginary frequencies)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	71	-0.202164	-0.013300	0.356033
2	7	-0.570051	2.529099	0.263164
3	7	0.470032	-2.531508	-0.386512
4	7	-0.931227	-1.212435	2.431394
5	7	0.561607	1.388187	-2.059085
6	8	-2.291768	0.057750	-0.116600
7	8	1.939791	0.442577	0.355485
8	15	-3.260478	-0.383718	-1.278781
9	15	2.895494	0.706382	-0.822747
10	8	-3.461479	0.857917	-2.135433
11	8	-4.546479	-1.019274	-0.785037
12	8	4.186400	1.386528	-0.398726
13	8	3.133303	-0.558809	-1.635905
14	6	-0.628853	5.257087	0.475319
15	6	0.924849	-4.391849	-1.780477
16	6	0.430833	-3.102216	-1.583860
17	6	-0.091955	-2.360185	-2.779826
18	6	-0.820221	-0.164864	-3.468348

19	6	-2.338512	-1.641291	-2.191429
20	6	1.487839	-4.488439	0.520114
21	6	0.982052	-3.219977	0.637826
22	6	0.976809	-2.561769	1.980134
23	6	1.462725	-5.088665	-0.727806
24	6	-0.800129	4.471421	1.597469
25	6	-0.746923	3.108212	1.444289
26	6	-0.844740	2.179783	2.612352
27	6	-0.445155	4.653152	-0.753434
28	6	-0.449253	3.272572	-0.829999
29	6	-0.376137	2.534195	-2.135787
30	6	0.490431	0.596599	-3.317870
31	6	1.976282	1.870260	-1.860342
32	1	-0.616691	6.325905	0.554163
33	1	0.888615	-4.812999	-2.763651
34	1	0.772771	-2.049868	-3.349892
35	1	-0.649575	-3.059573	-3.403651
36	1	-0.848076	-0.612442	-4.464972
37	1	-1.679658	0.474844	-3.376937
38	1	-2.323417	-2.528343	-1.575039
39	1	-2.828580	-1.909511	-3.127324
40	1	1.881606	-4.963739	1.390606
41	1	1.855349	-6.076140	-0.868800
42	1	-0.941170	4.870125	2.577760
43	1	-0.244581	5.232074	-1.627346
44	1	-1.368847	2.156142	-2.339639
45	1	-0.080861	3.215998	-2.930917
46	1	0.612424	1.270364	-4.169165
47	1	1.324190	-0.083796	-3.325478
48	1	1.960185	2.844531	-1.394909
49	1	2.465642	1.987407	-2.825945
50	8	0.425735	-1.420382	2.028907
51	8	1.504065	-3.169129	2.930325
52	8	-0.735825	0.943720	2.293878
53	8	-0.972213	2.636471	3.751667
54	8	4.419862	0.295166	-3.958330
55	1	3.843181	0.097886	-3.201257
56	1	5.305412	0.329990	-3.540980
57	8	6.290279	0.310314	-1.993744
58	1	5.714061	0.882345	-1.446426
59	1	6.185152	-0.584180	-1.621519
60	8	-0.217733	-0.530175	4.503538
61	1	0.145235	-0.785339	3.622473
62	8	-0.889775	-3.137936	4.574432
63	1	-0.775062	-2.183528	4.773961
64	1	-0.042933	-3.420610	4.190351
65	1	-0.915305	0.103494	4.272558
66	8	1.311996	1.700194	5.008876
67	1	0.530283	2.245867	4.801597
68	1	0.981076	0.779746	4.988379

69	8	4.223393	-2.204512	2.277042
70	1	4.389250	-2.451227	1.352385
71	1	3.378192	-2.553175	2.596161
72	8	2.161858	2.240657	2.496939
73	1	2.016542	2.017481	3.442591
74	1	2.143218	1.455254	1.925440
75	8	5.602254	-0.024838	1.499084
76	1	5.071612	0.636793	1.011515
77	1	5.028058	-0.578278	2.063793
78	8	3.408012	3.768387	0.750731
79	1	2.907250	3.399442	1.517827
80	1	3.881108	3.013548	0.346693
81	8	5.296497	-1.849913	-0.421073
82	1	5.563058	-1.184387	0.259517
83	1	4.484602	-1.527646	-0.865806
84	8	2.806788	-1.977866	-3.946353
85	1	2.890601	-1.743467	-3.002461
86	1	3.399617	-1.352205	-4.396747
87	8	2.553488	5.168388	-1.279856
88	1	2.792238	4.728573	-0.415527
89	1	3.249074	4.914791	-1.903753
90	8	-2.481841	-2.900415	2.333530
91	8	-4.406807	-1.107552	2.027525
92	8	-4.686154	2.752480	-0.680218
93	8	-6.656683	0.642752	-0.798307
94	8	-2.401645	-4.150123	0.123059
95	8	-4.599894	-3.809950	-1.537868
96	8	-5.901626	2.008987	-3.004019
97	8	-3.701949	1.532705	1.633531
98	1	-4.245964	-0.150593	2.146659
99	1	-4.189005	2.134074	1.043508
100	1	-3.068923	1.030627	1.086290
101	1	-6.155489	1.351975	-0.364207
102	1	-6.032304	-0.121748	-0.822441
103	1	-4.053024	2.139008	-1.121699
104	1	-5.300751	2.975777	-1.402138
105	1	-5.014466	1.599537	-3.021750
106	1	-6.407829	1.454695	-2.370746
107	1	-4.781375	-2.883586	-1.302667
108	1	-3.865618	-4.090913	-0.959374
109	1	-3.169243	-2.185374	2.341833
110	1	-1.992816	-3.006297	3.174847
111	1	-2.442884	-3.668339	1.012932
112	1	-1.591052	-4.668592	0.076466
113	1	-4.552668	-1.234575	1.067650

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