

Ln₂M complexes (M = Ru, Re) derived from a bismacrocyclic ligand containing a 4,4'-dimethyl-2,2'-bipyridyl bridging unit

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Supporting Information

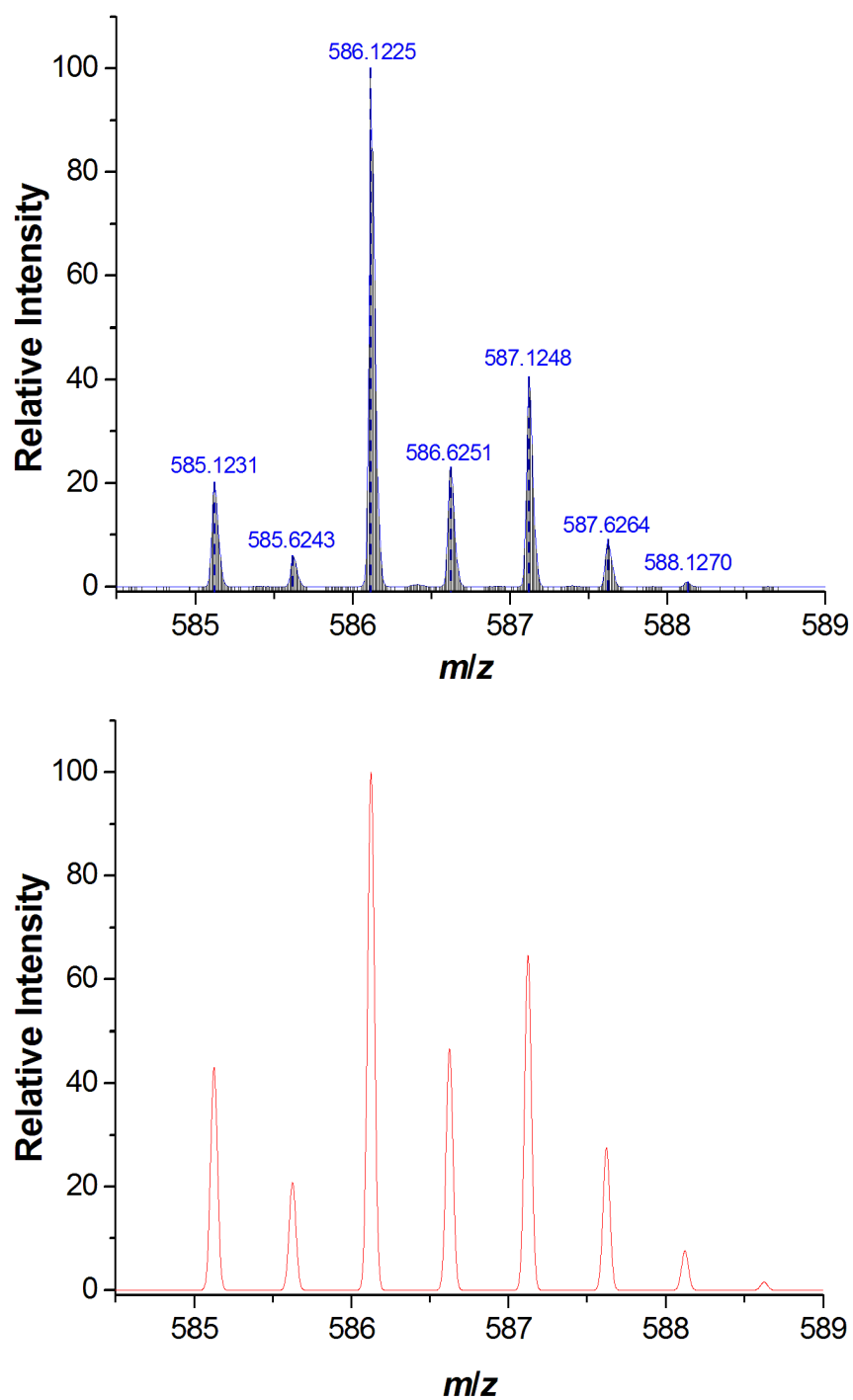


Figure S1 Observed (top) and theoretical (bottom) mass spectral isotopic distribution for the $[\text{Eu}_2\text{H}_2\mathbf{1}]^{2+}$ entity.

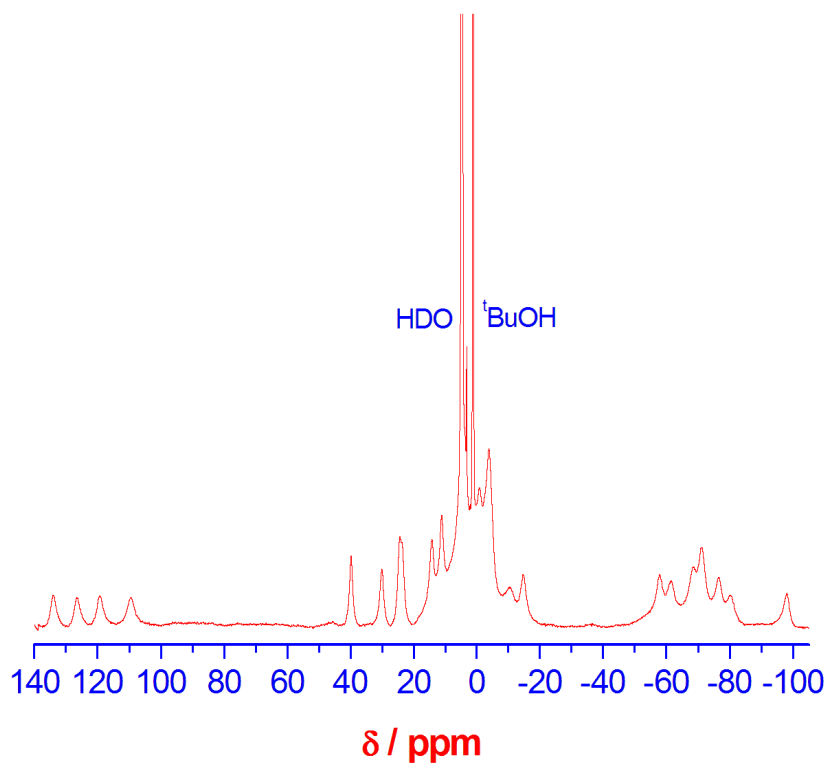
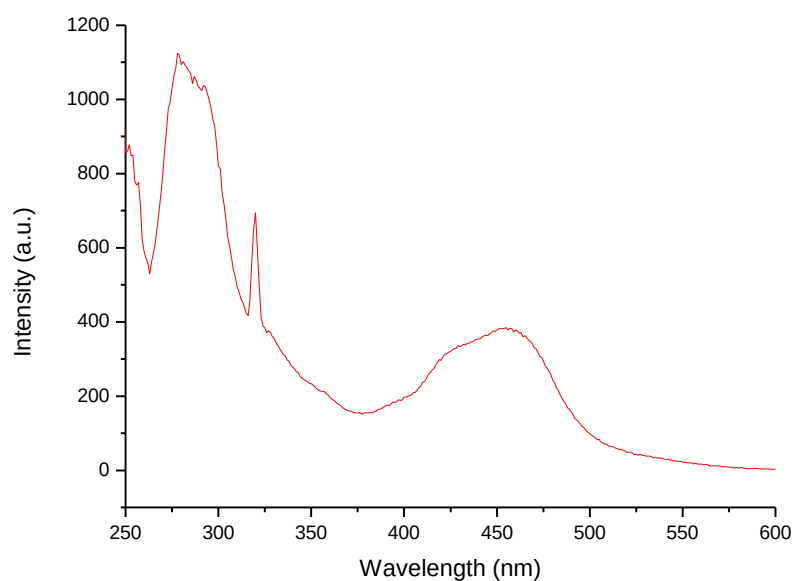


Figure S2 ^1H NMR spectrum (300 MHz) of $\text{Yb}_2\cdot\mathbf{1}$ recorded in D_2O solution at 298 K (pD $\sim$ 7.0).

a)



b)

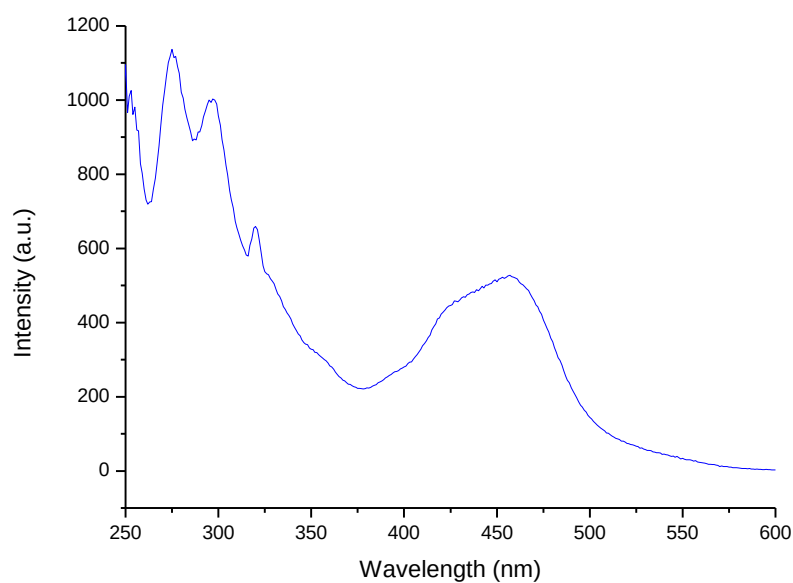


Figure S3 Excitation spectra of the complexes $[\text{Ln}_2.1.\text{Ru}(\text{Bpy})_2]^{2+}$ in 0.1 M TRIS buffered aqueous solutions (pH 7.4, 2×10^{-5} M); a) Ln = Eu, $\lambda_{\text{em}} = 641$ nm; b) Ln = Tb, $\lambda_{\text{em}} = 641$ nm.

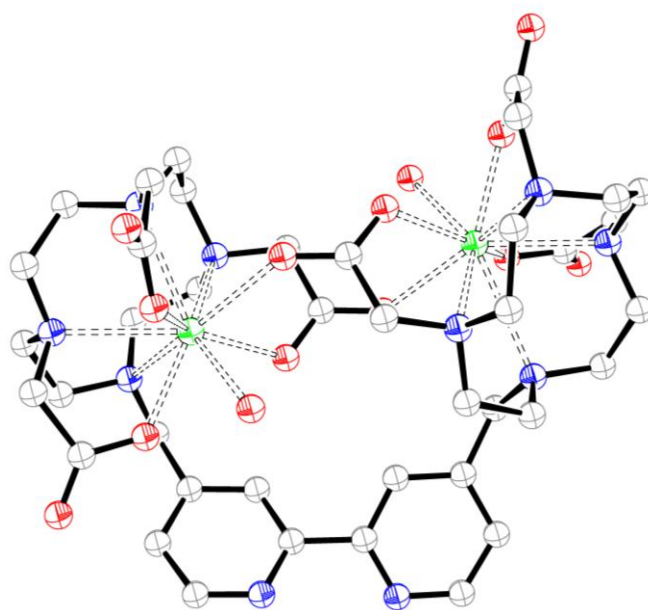


Figure S4 Optimized geometry of Yb₂.1·2H₂O obtained from DFT calculations (B3LYP). Hydrogen atoms are omitted for the sake of simplicity.

Yb₂.1·2H₂O [Δ(λλλ)] HF/3-21G (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-4.130194	2.052750	2.131204
2	1	-5.041658	2.406854	2.607253
3	1	-3.342990	2.132294	2.863323
4	6	-3.759275	2.969284	0.978316
5	6	-2.448544	3.395002	0.883747
6	6	-4.662397	3.472555	0.057524
7	6	-2.053045	4.241474	-0.139989
8	6	-4.202442	4.336177	-0.918988
9	1	-5.688570	3.177605	0.041664
10	1	-1.729914	3.050674	1.590320
11	1	-4.876354	4.724304	-1.653514
12	7	-2.929049	4.708863	-1.020586
13	6	2.691549	3.000910	0.612067
14	1	2.171767	2.301765	1.231814
15	1	3.403097	3.516261	1.239856
16	6	1.686123	4.008880	0.077768
17	6	0.343877	3.686506	0.120873
18	6	2.026633	5.274351	-0.382079
19	6	-0.617751	4.611153	-0.261925
20	1	0.039966	2.713038	0.429800
21	6	1.015504	6.128919	-0.782852
22	1	3.049005	5.595072	-0.417520
23	7	-0.275895	5.808758	-0.721773
24	1	1.244648	7.107995	-1.150923
25	8	-0.716896	-1.653830	-0.575313
26	6	0.488702	-1.529000	-0.937184
27	6	0.765846	-0.687957	-2.155959
28	8	1.474180	-2.028759	-0.314937
29	7	2.081447	0.018932	-2.046364
30	1	-0.030568	0.025685	-2.259524
31	1	0.730914	-1.338676	-3.024055
32	6	3.009875	-0.467172	-3.101462
33	6	1.819951	1.490123	-2.160856
34	8	4.193722	-2.256362	1.128921
35	8	3.914969	0.661763	2.108186
36	8	2.412764	-1.341531	2.658716
37	6	3.461586	-1.894310	-2.809205
38	6	3.027771	2.352980	-1.828144
39	6	4.695781	-3.279946	0.487014
40	6	5.127228	1.114913	2.273227
41	7	4.271923	-1.942407	-1.561209
42	7	3.490068	2.199052	-0.420208
43	6	4.262701	-3.312949	-0.976817
44	8	5.411401	-4.140666	0.953908
45	6	6.151719	0.359828	1.424282
46	8	5.466631	2.026962	3.001899
47	6	5.670267	-1.507311	-1.839790
48	6	4.941164	2.540854	-0.329443
49	1	4.899524	-3.987705	-1.536023
50	1	3.243254	-3.669868	-0.994960
51	7	5.650291	0.149669	0.031981
52	1	7.097470	0.887982	1.426831
53	1	6.277144	-0.616076	1.873086
54	6	6.390334	-0.979710	-0.601115
55	6	5.829943	1.385615	-0.782636
56	1	-1.484061	-4.305417	-0.903954

57	6	-2.459931	-3.867968	-1.035255
58	7	-2.908276	-3.226409	0.246512
59	6	-2.361024	-2.892079	-2.211884
60	1	-3.140568	-4.669750	-1.307232
61	6	-4.295842	-3.637512	0.588327
62	6	-1.957002	-3.574568	1.346089
63	8	-1.646244	-3.172085	-3.156830
64	8	-3.074705	-1.804734	-2.083100
65	6	-5.314394	-2.978052	-0.333723
66	6	-2.124629	-2.680522	2.573757
67	7	-5.305835	-1.496422	-0.177353
68	7	-1.882990	-1.248750	2.246055
69	8	-1.186945	0.772697	0.750623
70	8	-4.237258	0.778878	-1.163937
71	8	-1.964098	0.567284	-2.213218
72	6	-6.063540	-1.086190	1.035663
73	6	-5.902325	-0.855793	-1.387238
74	6	-2.480670	-0.346021	3.272389
75	6	-0.420066	-0.974645	2.168624
76	6	-0.167810	0.176152	1.214705
77	6	-5.493131	0.611875	-1.459867
78	6	-5.754896	0.340494	1.497304
79	1	-6.981864	-0.946140	-1.386008
80	1	-5.486098	-1.345672	-2.254192
81	6	-3.983167	-0.181550	3.094663
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83	1	0.119379	-1.825589	1.800560
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85	8	-6.294480	1.477513	-1.762680
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87	1	-2.636861	1.267394	-2.179991
88	1	-2.315082	-0.181975	-2.734756
89	1	3.076192	-2.042963	2.509261
90	1	2.865484	-0.563905	3.031818
91	1	-4.498916	-3.364268	1.611748
92	1	-4.391860	-4.719581	0.519152
93	1	-5.070819	-3.197000	-1.359126
94	1	-6.306523	-3.375650	-0.127213
95	1	-5.851259	-1.787011	1.827405
96	1	-7.131774	-1.151004	0.836145
97	1	-6.370034	0.544604	2.374631
98	1	-6.041175	1.047028	0.740266
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100	1	-4.400272	0.333388	3.958672
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102	1	-2.268921	-0.731603	4.268231
103	1	-3.119424	-2.777067	2.980941
104	1	-1.432075	-3.009692	3.345766
105	1	-0.964655	-3.457035	0.949159
106	1	-2.091924	-4.613639	1.643678
107	1	3.865605	0.186217	-3.146779
108	1	2.518165	-0.429570	-4.071698
109	1	4.032510	-2.279786	-3.651669
110	1	2.603387	-2.531767	-2.674906
111	1	1.488456	1.721697	-3.171830
112	1	1.012691	1.718054	-1.488258
113	1	3.852683	2.098844	-2.476647
114	1	2.774381	3.384843	-2.036945
115	1	6.237998	-2.340924	-2.247853
116	1	5.645647	-0.742469	-2.600111
117	1	6.511813	-1.761844	0.127741

118	1	7.387638	-0.652650	-0.893411
119	1	6.870268	1.703863	-0.728426
120	1	5.618381	1.146875	-1.812896
121	1	5.179425	2.803125	0.685682
122	1	5.166080	3.409403	-0.947207
123	70	-2.805912	-0.610686	-0.192155
124	70	3.096549	-0.471059	0.368190

E(RB+HF-LYP) = -3202.4266385 Hartree
Zero-point correction = 1.100099 Hartree/particle
Sum of electronic and thermal Energies = -3201.270302 Hartree
Sum of electronic and thermal Enthalpies = -3201.269357 Hartree
Sum of electronic and thermal Free Energies = -3201.410122 Hartree

Yb₂.1 · 2H₂O [Δ(λλλλ)] B3LYP/6-31G(d)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-4.072276	2.319149	2.233955
2	1	-4.976244	2.718872	2.722690
3	1	-3.267577	2.403974	2.968168
4	6	-3.690455	3.197121	1.057468
5	6	-2.351313	3.554928	0.898075
6	6	-4.603533	3.742186	0.152609
7	6	-1.955289	4.387931	-0.156948
8	6	-4.124194	4.575977	-0.861700
9	1	-5.665102	3.524687	0.202940
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12	7	-2.839356	4.900464	-1.028949
13	6	2.840762	3.108829	0.536056
14	1	2.341922	2.450663	1.244448
15	1	3.571922	3.686945	1.107391
16	6	1.819548	4.086056	-0.019695
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19	6	-0.508293	4.715827	-0.332263
20	1	0.156563	2.817787	0.453473
21	6	1.126088	6.184169	-0.975272
22	1	3.191491	5.653224	-0.643632
23	7	-0.176001	5.902826	-0.867283
24	1	1.365829	7.156412	-1.404492
25	8	-0.690793	-1.829282	-0.784373
26	6	0.523117	-1.563352	-1.012729
27	6	0.819706	-0.581688	-2.145021
28	8	1.497175	-2.044569	-0.359273
29	7	2.160160	0.062973	-2.070531
30	1	0.035578	0.173178	-2.140862
31	1	0.698781	-1.123697	-3.093856
32	6	3.042739	-0.470521	-3.133381
33	6	1.986544	1.536074	-2.212927
34	8	4.269851	-2.361712	1.096073
35	8	3.997591	0.621064	2.127250
36	8	2.450983	-1.440428	2.679325
37	6	3.504302	-1.897393	-2.850857
38	6	3.221781	2.353730	-1.849098
39	6	4.678989	-3.408871	0.425953
40	6	5.246499	0.924863	2.364947
41	7	4.320189	-1.982052	-1.618698

42	7	3.620535	2.225825	-0.430974
43	6	4.315829	-3.359480	-1.068955
44	8	5.259534	-4.378777	0.884067
45	6	6.245750	0.215838	1.428643
46	8	5.658166	1.659293	3.249878
47	6	5.708259	-1.537319	-1.889963
48	6	5.072642	2.487411	-0.280220
49	1	4.983613	-4.025247	-1.632610
50	1	3.296452	-3.748497	-1.145738
51	7	5.747607	0.069415	0.034758
52	1	7.211668	0.738048	1.457005
53	1	6.385999	-0.789395	1.837013
54	6	6.450707	-1.044137	-0.648550
55	6	5.959763	1.326068	-0.721817
56	1	-1.698104	-4.072140	-0.856946
57	6	-2.783922	-3.978674	-0.789521
58	7	-3.101441	-3.194175	0.436232
59	6	-3.230228	-3.307064	-2.104995
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62	6	-2.140372	-3.518749	1.522772
63	8	-3.413380	-4.001901	-3.091150
64	8	-3.336195	-2.005297	-2.041822
65	6	-5.549018	-2.791156	0.000523
66	6	-2.166890	-2.513834	2.676774
67	7	-5.417845	-1.314177	0.039397
68	7	-1.891580	-1.123252	2.237956
69	8	-1.086588	0.729307	0.461272
70	8	-4.197265	0.842839	-1.143337
71	8	-2.089376	0.280905	-2.531565
72	6	-6.081578	-0.791533	1.256478
73	6	-6.018805	-0.687128	-1.165696
74	6	-2.385244	-0.145719	3.243253
75	6	-0.431503	-0.913800	2.083697
76	6	-0.116716	0.200955	1.084547
77	6	-5.472407	0.730692	-1.409192
78	6	-5.710020	0.636363	1.656402
79	1	-7.115087	-0.660075	-1.103631
80	1	-5.728375	-1.284082	-2.034552
81	6	-3.888258	0.104935	3.187540
82	1	0.050616	-0.703020	3.046272
83	1	0.045702	-1.815991	1.701588
84	8	1.093216	0.511314	0.893000
85	8	-6.202230	1.612401	-1.838409
86	7	-4.284724	0.853737	1.977491
87	1	-2.828600	0.924396	-2.508773
88	1	-2.470260	-0.519684	-2.954501
89	1	3.135834	-2.135626	2.569619
90	1	2.933908	-0.684851	3.075327
91	1	-4.607047	-3.146698	1.903402
92	1	-4.676576	-4.562332	0.864025
93	1	-5.455506	-3.119020	-1.034789
94	1	-6.547229	-3.108418	0.343697
95	1	-5.869390	-1.477410	2.080467
96	1	-7.175701	-0.817479	1.119073
97	1	-6.344949	0.901913	2.522859
98	1	-5.979902	1.324266	0.854629
99	1	-4.413211	-0.851836	3.204129
100	1	-4.197866	0.634026	4.105838
101	1	-1.861250	0.795307	3.062511
102	1	-2.103663	-0.478510	4.255883

103	1	-3.142899	-2.527526	3.169353
104	1	-1.436907	-2.834813	3.436617
105	1	-1.145888	-3.527614	1.073864
106	1	-2.328909	-4.526196	1.928790
107	1	3.910078	0.187120	-3.230942
108	1	2.526269	-0.446006	-4.107573
109	1	4.057058	-2.278473	-3.725141
110	1	2.633784	-2.542751	-2.719184
111	1	1.687474	1.787819	-3.243817
112	1	1.164575	1.824325	-1.558121
113	1	4.070207	2.042382	-2.463852
114	1	3.024616	3.398730	-2.124650
115	1	6.289860	-2.357081	-2.342063
116	1	5.672631	-0.741914	-2.638745
117	1	6.563721	-1.861185	0.063427
118	1	7.467322	-0.739416	-0.948298
119	1	7.010972	1.647433	-0.624850
120	1	5.800311	1.117409	-1.783046
121	1	5.276577	2.710566	0.767044
122	1	5.376198	3.380423	-0.854000
123	70	-2.795980	-0.679647	-0.313978
124	70	3.162601	-0.537578	0.389913

E (RB+HF-LYP) = -3239.2024987 Hartree

Yb₂.1·2H₂O [Δ(δδδδ)] HF/3-21G (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-4.399709	2.342424	1.561443
2	1	-5.418045	2.345125	1.213123
3	1	-4.393829	2.857940	2.520099
4	6	-3.606419	3.161380	0.555141
5	6	-2.336396	3.648311	0.802382
6	6	-4.232286	3.558442	-0.620204
7	6	-1.717659	4.461465	-0.137906
8	6	-3.573161	4.419259	-1.472696
9	1	-5.192058	3.177471	-0.897135
10	1	-1.812622	3.394632	1.698723
11	1	-4.040509	4.753174	-2.375692
12	7	-2.340086	4.857580	-1.239630
13	6	2.892020	2.882666	0.629746
14	1	2.430284	2.246474	1.355455
15	1	3.805203	3.256407	1.061876
16	6	1.962605	4.039766	0.318325
17	6	0.598588	3.813718	0.337838
18	6	2.394718	5.317663	0.003739
19	6	-0.283206	4.819284	-0.004610
20	1	0.219109	2.840021	0.543380
21	6	1.447976	6.284915	-0.296610
22	1	3.437242	5.565521	-0.007617
23	7	0.141967	6.040286	-0.318165
24	1	1.749857	7.283557	-0.537666
25	8	-0.774242	-1.680099	-0.565505
26	6	0.430676	-1.513464	-0.912855
27	6	0.702453	-0.517016	-2.020504
28	8	1.426215	-2.042092	-0.333347
29	7	2.162935	-0.306877	-2.176194
30	1	0.201085	0.395816	-1.759540

31	1	0.253585	-0.864742	-2.944194
32	6	2.694361	-1.386175	-3.059743
33	6	2.441499	1.039591	-2.745997
34	8	4.107146	-2.382927	1.037608
35	8	4.017107	0.479761	2.103494
36	8	2.350199	-1.415279	2.560092
37	6	4.193597	-1.582217	-2.896405
38	1	2.177508	-2.298185	-2.811591
39	1	2.465051	-1.155421	-4.098377
40	6	2.284922	2.143877	-1.702342
41	1	1.757730	1.242194	-3.567970
42	1	3.438674	1.034526	-3.157001
43	6	4.255561	-3.502981	0.370395
44	6	5.279326	0.465349	2.460833
45	7	4.541886	-1.910480	-1.493373
46	1	4.714992	-0.679457	-3.177120
47	1	4.529523	-2.371446	-3.567389
48	7	3.267293	2.022585	-0.580833
49	1	2.388101	3.107724	-2.192423
50	1	1.298706	2.096272	-1.284053
51	6	4.174206	-3.308168	-1.144925
52	8	4.401777	-4.608622	0.842237
53	6	6.207648	-0.026393	1.346527
54	8	5.722458	0.756936	3.550165
55	6	6.002200	-1.732856	-1.256420
56	6	4.635072	2.378445	-1.049234
57	1	4.817847	-4.025567	-1.643012
58	1	3.150616	-3.493869	-1.429070
59	7	5.646234	0.367760	0.025966
60	1	7.202239	0.379771	1.493515
61	1	6.241583	-1.103478	1.411014
62	6	6.380167	-0.267493	-1.096006
63	1	6.567733	-2.167259	-2.079491
64	1	6.266643	-2.275294	-0.363905
65	6	5.701875	1.853267	-0.097204
66	1	4.732545	3.457184	-1.150008
67	1	4.790155	1.954076	-2.028709
68	1	6.150310	0.275369	-2.001110
69	1	7.454533	-0.187184	-0.937652
70	1	5.563700	2.278646	0.882675
71	1	6.686812	2.160679	-0.443942
72	1	-1.534644	-3.884076	-0.258340
73	6	-2.557853	-3.858739	-0.586158
74	7	-3.393627	-3.103348	0.390434
75	6	-2.572933	-3.161859	-1.955162
76	1	-2.914039	-4.879762	-0.689728
77	6	-4.815608	-3.459811	0.106901
78	6	-3.033073	-3.407859	1.800633
79	8	-1.990665	-3.672355	-2.890147
80	8	-3.197157	-2.007550	-1.968450
81	6	-5.808156	-2.481003	0.710241
82	1	-5.020830	-4.462224	0.479725
83	1	-4.934102	-3.476680	-0.963053
84	6	-1.737550	-2.719765	2.224206
85	1	-3.846609	-3.091070	2.436087
86	1	-2.918323	-4.481814	1.937653
87	7	-5.569977	-1.102539	0.228912
88	1	-5.727056	-2.481811	1.787854
89	1	-6.820236	-2.800908	0.466041
90	7	-1.805089	-1.225139	2.135128
91	1	-0.936449	-3.030208	1.576423

92	1	-1.488280	-3.021795	3.239560
93	8	-1.167275	0.835236	0.486539
94	8	-4.324665	0.680662	-1.322526
95	8	-2.075699	0.296792	-2.390787
96	6	-6.225588	-0.116039	1.133572
97	6	-6.067445	-0.882287	-1.161234
98	6	-2.590736	-0.627548	3.247182
99	6	-0.413996	-0.687563	2.157223
100	6	-0.166558	0.310314	1.057713
101	6	-5.597039	0.519836	-1.544859
102	6	-5.312083	0.229791	2.293941
103	1	-6.479043	0.762451	0.563367
104	1	-7.160754	-0.522159	1.514331
105	1	-7.148197	-0.943019	-1.207779
106	1	-5.609756	-1.601326	-1.821355
107	6	-3.035201	0.807651	2.940101
108	1	-1.986765	-0.612947	4.151917
109	1	-3.438169	-1.257759	3.453916
110	1	-0.196538	-0.212006	3.108815
111	1	0.308193	-1.473033	2.053749
112	8	1.040079	0.547654	0.740118
113	8	-6.372792	1.373741	-1.938757
114	7	-4.043090	0.885243	1.836923
115	1	-5.830106	0.880057	2.997211
116	1	-5.073229	-0.676391	2.820980
117	1	-3.454446	1.241016	3.847995
118	1	-2.184243	1.396378	2.647248
119	1	-2.776748	0.966472	-2.453431
120	1	-2.401642	-0.531320	-2.799661
121	1	2.968083	-2.151927	2.376471
122	1	2.847004	-0.693340	2.984543
123	70	3.113285	-0.503012	0.307187
124	70	-2.870674	-0.596430	-0.231585

E(RB+HF-LYP) = -3202.4201527 Hartree
Zero-point correction = 1.099373 Hartree/particle
Sum of electronic and thermal Energies = -3201.264299 Hartree
Sum of electronic and thermal Enthalpies = -3201.263355 Hartree
Sum of electronic and thermal Free Energies = -3201.405298 Hartree

Yb₂.1 · 2H₂O [Δ(δδδδ)] B3LYP/6-31G(d)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-4.321211	2.481101	1.891277
2	1	-5.395760	2.583422	1.726678
3	1	-4.118131	2.956758	2.864490
4	6	-3.640994	3.282607	0.796379
5	6	-2.332106	3.755816	0.904586
6	6	-4.368041	3.678293	-0.331336
7	6	-1.793536	4.558387	-0.113424
8	6	-3.770531	4.529781	-1.260932
9	1	-5.380683	3.328965	-0.504946
10	1	-1.724806	3.511998	1.770830
11	1	-4.333457	4.864115	-2.130431
12	7	-2.511933	4.966917	-1.170876
13	6	2.886425	2.988942	0.481554
14	1	2.431009	2.375540	1.255593
15	1	3.806337	3.395022	0.904993

16	6	1.940447	4.124767	0.146463
17	6	0.566276	3.902626	0.248642
18	6	2.348113	5.396601	-0.267697
19	6	-0.342197	4.903803	-0.108502
20	1	0.201463	2.925807	0.539522
21	6	1.367900	6.347524	-0.575069
22	1	3.400799	5.656598	-0.346703
23	7	0.052130	6.121579	-0.519096
24	1	1.663490	7.347738	-0.889689
25	8	-0.741051	-1.834265	-0.670903
26	6	0.473986	-1.605551	-0.927080
27	6	0.783133	-0.617982	-2.053124
28	8	1.449939	-2.087176	-0.275431
29	7	2.235865	-0.373048	-2.187926
30	1	0.259090	0.307123	-1.817525
31	1	0.347893	-0.979669	-2.994860
32	6	2.811191	-1.450200	-3.032037
33	6	2.480870	0.959175	-2.787543
34	8	4.197569	-2.392706	1.118072
35	8	4.030956	0.545698	2.135260
36	8	2.381912	-1.416497	2.661802
37	6	4.313111	-1.627908	-2.849102
38	1	2.301567	-2.378580	-2.769015
39	1	2.592568	-1.260566	-4.095544
40	6	2.318236	2.107862	-1.791974
41	1	1.790288	1.136353	-3.627579
42	1	3.486295	0.956811	-3.216617
43	6	4.396914	-3.505254	0.452776
44	6	5.295677	0.582263	2.480758
45	7	4.672226	-1.920195	-1.449084
46	1	4.834039	-0.714789	-3.152758
47	1	4.663937	-2.425530	-3.525528
48	7	3.282642	2.068573	-0.662804
49	1	2.393458	3.055516	-2.347170
50	1	1.316075	2.069703	-1.368187
51	6	4.364144	-3.319720	-1.076629
52	8	4.572037	-4.612993	0.927686
53	6	6.258931	0.134538	1.361894
54	8	5.737108	0.897896	3.572462
55	6	6.115618	-1.679911	-1.213253
56	6	4.645367	2.405478	-1.128238
57	1	5.057211	-4.029690	-1.550166
58	1	3.351449	-3.567808	-1.404167
59	7	5.703782	0.451415	0.025147
60	1	7.242362	0.601117	1.515706
61	1	6.373780	-0.949396	1.453458
62	6	6.461185	-0.203741	-1.059286
63	1	6.718217	-2.108436	-2.031365
64	1	6.397462	-2.215981	-0.305256
65	6	5.720676	1.921842	-0.161163
66	1	4.757078	3.491472	-1.281050
67	1	4.805839	1.944816	-2.106303
68	1	6.244910	0.328074	-1.991306
69	1	7.547691	-0.107146	-0.895232
70	1	5.574196	2.386540	0.815677
71	1	6.708946	2.255657	-0.517350
72	1	-1.728438	-3.986770	-0.299108
73	6	-2.786650	-3.960049	-0.561326
74	7	-3.521059	-3.129049	0.428603
75	6	-2.884972	-3.363735	-1.984507
76	1	-3.162418	-4.992944	-0.568614

77	6	-4.969869	-3.394743	0.231818
78	6	-3.113804	-3.425200	1.821703
79	8	-2.576466	-4.053642	-2.940574
80	8	-3.284964	-2.114857	-2.018290
81	6	-5.882636	-2.325844	0.816846
82	1	-5.237681	-4.373066	0.663310
83	1	-5.142038	-3.468182	-0.842985
84	6	-1.802145	-2.748848	2.217890
85	1	-3.920438	-3.103368	2.487508
86	1	-3.004386	-4.511135	1.973793
87	7	-5.582775	-0.976756	0.304330
88	1	-5.782028	-2.303887	1.906574
89	1	-6.930085	-2.605491	0.611186
90	7	-1.836678	-1.260840	2.114244
91	1	-1.007812	-3.092666	1.554746
92	1	-1.535485	-3.063044	3.239776
93	8	-1.154251	0.781429	0.384223
94	8	-4.273132	0.720578	-1.352588
95	8	-2.058438	0.165787	-2.563619
96	6	-6.176409	0.047010	1.197684
97	6	-6.112371	-0.761175	-1.063947
98	6	-2.575646	-0.668691	3.252693
99	6	-0.443692	-0.740295	2.102876
100	6	-0.169754	0.285949	1.011721
101	6	-5.542079	0.556285	-1.623835
102	6	-5.302306	0.343102	2.407268
103	1	-6.324451	0.960802	0.618070
104	1	-7.176811	-0.272627	1.533074
105	1	-7.210857	-0.726125	-1.073179
106	1	-5.777260	-1.575159	-1.713368
107	6	-2.999240	0.790760	3.056945
108	1	-1.952611	-0.714288	4.160962
109	1	-3.445736	-1.293087	3.461686
110	1	-0.181087	-0.290698	3.069695
111	1	0.266417	-1.551925	1.966505
112	8	1.040985	0.578201	0.778447
113	8	-6.252829	1.333693	-2.243052
114	7	-4.036341	1.007106	2.025058
115	1	-5.868564	0.952524	3.132188
116	1	-5.080296	-0.594502	2.917387
117	1	-3.343186	1.167381	4.038309
118	1	-2.127966	1.386693	2.775549
119	1	-2.816922	0.782957	-2.631037
120	1	-2.401660	-0.675728	-2.941236
121	1	3.035815	-2.140973	2.539935
122	1	2.900952	-0.689694	3.067331
123	70	3.148492	-0.540032	0.370281
124	70	-2.854602	-0.672248	-0.335395

E (RB+HF-LYP) = -3239.1968356 Hartree

[Yb₂.1.Ru(Bpy)₂]²⁺·2H₂O [Δ(λλλ)] HF/3-21G (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-4.384322	-1.192574	0.474080
2	6	-4.901666	-0.166887	1.431959
3	6	-6.141109	-0.650739	2.190942
4	7	-7.295503	-0.956144	1.302182

5	6	-8.366622	-1.672971	2.063698
6	6	-8.009813	-3.140615	2.309726
7	7	-7.694591	-3.897777	1.057704
8	6	-6.840922	-5.079984	1.387841
9	6	-5.369270	-4.670131	1.511153
10	7	-4.808850	-4.132443	0.230096
11	6	-3.467425	-3.522948	0.442116
12	6	-3.530785	-2.185013	1.178914
13	6	-7.857219	0.286446	0.676229
14	6	-6.944742	0.753612	-0.455679
15	8	-6.551371	1.917464	-0.516223
16	8	-6.582937	-0.201720	-1.249465
17	6	-8.959968	-4.314350	0.359896
18	6	-9.607199	-3.102437	-0.327963
19	8	-10.800571	-2.920247	-0.283113
20	8	-8.718259	-2.323383	-0.902954
21	6	-4.713592	-5.239242	-0.778472
22	6	-6.054432	-5.417694	-1.500495
23	8	-6.530548	-6.518770	-1.670841
24	8	-6.562683	-4.268920	-1.849335
25	1	-7.980314	1.073266	1.409188
26	1	-8.810200	0.023921	0.240373
27	1	-9.658257	-4.758357	1.057042
28	1	-8.703464	-5.033384	-0.406506
29	1	-3.984244	-4.955656	-1.526538
30	1	-4.405314	-6.167592	-0.316199
31	1	-5.138145	0.736243	0.905353
32	1	-4.130416	0.081340	2.158225
33	1	-6.423922	0.117670	2.908042
34	1	-5.900932	-1.541624	2.751833
35	1	-8.523632	-1.189143	3.025625
36	1	-9.286684	-1.596081	1.511699
37	1	-8.840007	-3.618767	2.822222
38	1	-7.154949	-3.203745	2.967120
39	1	-7.158139	-5.523356	2.327883
40	1	-6.965559	-5.829605	0.625364
41	1	-5.270996	-3.912053	2.273018
42	1	-4.784496	-5.531755	1.824935
43	1	-3.027274	-3.378890	-0.534293
44	1	-2.821042	-4.202044	0.995710
45	1	-3.935102	-2.330402	2.168665
46	1	-2.520557	-1.801956	1.310921
47	6	-3.718449	-0.596818	-0.738312
48	1	-3.131606	-1.370384	-1.210855
49	1	-4.506531	-0.311662	-1.409883
50	6	-2.849570	0.635958	-0.503049
51	6	-1.486045	0.561338	-0.251541
52	6	-3.423393	1.896663	-0.625580
53	6	-0.733230	1.716957	-0.124976
54	6	-2.624478	3.006964	-0.475624
55	1	-4.474256	2.016372	-0.822959
56	1	-1.015816	-0.394748	-0.177720
57	1	-3.034787	3.988959	-0.558076
58	7	-1.313020	2.922075	-0.236746
59	8	6.525723	-6.520367	1.672129
60	6	6.051173	-5.418867	1.500233
61	6	4.710857	-5.239588	0.777527
62	8	6.560657	-4.270387	1.848174
63	7	4.807175	-4.132979	-0.231047
64	1	3.981339	-4.955511	1.525257
65	1	4.402209	-6.167831	0.315262

66	6	5.368770	-4.670896	-1.511518
67	6	3.466012	-3.523513	-0.444619
68	8	6.581884	-0.202207	1.248517
69	8	8.717301	-2.324121	0.903691
70	8	5.909883	-2.050155	2.905732
71	6	6.840331	-5.080853	-1.387108
72	1	5.271091	-3.912945	-2.273585
73	1	4.784229	-5.532561	-1.825643
74	6	3.530448	-2.185353	-1.180856
75	1	3.024442	-3.379841	0.531209
76	1	2.820382	-4.202404	-0.999347
77	6	6.944455	0.752963	0.454958
78	6	9.606327	-3.103580	0.329443
79	7	7.694127	-3.898730	-1.057005
80	1	7.157982	-5.524678	-2.326797
81	1	6.964407	-5.830248	-0.624306
82	7	4.384029	-1.193518	-0.475207
83	1	3.935371	-2.330609	-2.170374
84	1	2.520502	-1.801748	-1.313408
85	6	7.857399	0.285407	-0.676379
86	8	6.551406	1.916954	0.515220
87	6	8.959157	-4.315395	-0.358674
88	8	10.799790	-2.921805	0.285276
89	6	8.009964	-3.141950	-2.309096
90	6	4.901908	-0.167606	-1.432632
91	6	3.717898	-0.598195	0.737287
92	7	7.295622	-0.957173	-1.302214
93	1	7.981009	1.072012	-1.409481
94	1	8.810117	0.022745	-0.240023
95	1	9.657671	-4.759595	-1.055468
96	1	8.702196	-5.034277	0.407712
97	6	8.366850	-1.674309	-2.063270
98	1	8.840306	-3.620349	-2.821121
99	1	7.155376	-3.205126	-2.966835
100	6	6.141496	-0.651606	-2.191301
101	1	5.138349	0.735384	-0.905786
102	1	4.130929	0.080906	-2.159087
103	1	3.130603	-1.371858	1.209160
104	1	4.505839	-0.313592	1.409320
105	6	2.849474	0.634945	0.502375
106	1	8.524262	-1.190708	-3.025243
107	1	9.286727	-1.597432	-1.510968
108	1	6.424616	0.116747	-2.908341
109	1	5.901318	-1.542452	-2.752242
110	6	1.485939	0.560807	0.250776
111	6	3.423702	1.895438	0.625211
112	6	0.733491	1.716696	0.124445
113	1	1.015418	-0.395118	0.176720
114	6	2.625134	3.006019	0.475468
115	1	4.474597	2.014845	0.822614
116	7	1.313663	2.921593	0.236497
117	1	3.035738	3.987875	0.558153
118	44	0.000577	4.619526	0.000039
119	1	-0.626166	3.343990	-2.816320
120	6	0.144727	4.038816	-3.065918
121	6	0.601607	4.167220	-4.360263
122	6	1.603710	5.672590	-2.298429
123	6	1.601730	5.086260	-4.615323
124	1	0.183419	3.567260	-5.140493
125	6	2.082993	6.452875	-1.128411
126	6	2.107995	5.844702	-3.575134

127	1	1.983623	5.215664	-5.607236
128	6	3.056908	7.429656	-1.224023
129	1	2.880960	6.554429	-3.767966
130	6	1.890745	6.828152	1.152652
131	6	3.448899	8.114526	-0.087230
132	1	3.510640	7.662683	-2.161147
133	6	2.857265	7.811232	1.123629
134	1	1.404989	6.557516	2.063612
135	1	4.204018	8.870780	-0.151145
136	1	3.135375	8.319070	2.022614
137	7	0.633162	4.774096	-2.064319
138	7	1.516754	6.166299	0.055622
139	1	0.626804	3.343019	2.816171
140	6	-0.143910	4.038001	3.065883
141	6	-0.600900	4.166155	4.360216
142	6	-1.600784	5.085407	4.615438
143	1	-0.182976	3.565837	5.140313
144	6	-1.602335	5.672432	2.298716
145	6	-2.106708	5.844313	3.575417
146	1	-1.982759	5.214619	5.607343
147	6	-2.081234	6.453251	1.128888
148	1	-2.879496	6.554198	3.768375
149	6	-3.054643	7.430507	1.224763
150	6	-3.446295	8.115881	0.088155
151	1	-3.508233	7.663532	2.161956
152	6	-1.888785	6.829057	-1.152070
153	6	-2.854820	7.812609	-1.122784
154	1	-4.201021	8.872508	0.152280
155	1	-1.403174	6.558435	-2.063110
156	1	-3.132671	8.320825	-2.021635
157	7	-0.632006	4.773727	2.064452
158	7	-1.515094	6.166737	-0.055221
159	8	-5.903572	-2.049644	-2.904048
160	1	-6.188171	-2.850261	-3.372084
161	1	-6.270278	-1.229360	-3.262599
162	1	6.194004	-2.851043	3.373533
163	1	6.277427	-1.230201	3.264086
164	70	-6.599700	-2.386084	-0.686384
165	70	6.598759	-2.386896	0.686479

E(RB+HF-LYP) = -4274.2812975 Hartree
Zero-point correction = 1.449369 Hartree/particle
Sum of electronic and thermal Energies = -4272.754590 Hartree
Sum of electronic and thermal Enthalpies = -4272.753646 Hartree
Sum of electronic and thermal Free Energies = -4272.950440 Hartree

[Yb₂.1.Ru(Bpy)₂]²⁺·2H₂O [Δ(λλλ)] B3LYP/6-31G(d)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-4.419789	-1.331770	0.512171
2	6	-4.820538	-0.387581	1.584831
3	6	-6.047257	-0.851327	2.377728
4	7	-7.277447	-1.000542	1.569246
5	6	-8.313457	-1.743830	2.338201
6	6	-8.046536	-3.250973	2.376989
7	7	-7.910275	-3.879333	1.034122
8	6	-7.118075	-5.133587	1.133823
9	6	-5.610358	-4.869597	1.192882

10	7	-5.064549	-4.207904	-0.023201
11	6	-3.689092	-3.719131	0.222067
12	6	-3.623646	-2.445826	1.068209
13	6	-7.790113	0.327694	1.124768
14	6	-6.956773	0.879453	-0.048250
15	8	-6.569359	2.051842	-0.041086
16	8	-6.684353	0.004106	-0.963606
17	6	-9.255892	-4.128867	0.432475
18	6	-9.886032	-2.838048	-0.133321
19	8	-11.081030	-2.642173	-0.043651
20	8	-9.007454	-2.033517	-0.696779
21	6	-5.073736	-5.166220	-1.164892
22	6	-6.417407	-5.202797	-1.925360
23	8	-6.802921	-6.248422	-2.414075
24	8	-6.998118	-4.034610	-1.996741
25	1	-7.804684	1.050000	1.951513
26	1	-8.810326	0.183297	0.758675
27	1	-9.938313	-4.589758	1.156710
28	1	-9.127812	-4.813958	-0.411321
29	1	-4.321291	-4.841633	-1.892280
30	1	-4.804154	-6.179274	-0.840823
31	1	-5.028781	0.586608	1.149610
32	1	-3.993900	-0.237438	2.298647
33	1	-6.212000	-0.127759	3.193776
34	1	-5.836180	-1.812545	2.855097
35	1	-8.373482	-1.372671	3.373457
36	1	-9.280925	-1.547342	1.876217
37	1	-8.860412	-3.733423	2.938539
38	1	-7.129351	-3.448877	2.939562
39	1	-7.403264	-5.708775	2.027712
40	1	-7.355678	-5.762642	0.274348
41	1	-5.384688	-4.237147	2.056646
42	1	-5.094223	-5.828445	1.362016
43	1	-3.236240	-3.527879	-0.755834
44	1	-3.067432	-4.491845	0.705180
45	1	-3.999614	-2.651671	2.073476
46	1	-2.564626	-2.163637	1.199177
47	6	-3.767561	-0.676328	-0.667695
48	1	-3.180879	-1.441188	-1.184024
49	1	-4.566779	-0.354043	-1.338148
50	6	-2.889827	0.545086	-0.423682
51	6	-1.507058	0.467169	-0.225083
52	6	-3.461328	1.827096	-0.476789
53	6	-0.733638	1.626832	-0.091980
54	6	-2.644365	2.939521	-0.328811
55	1	-4.534400	1.970313	-0.625763
56	1	-1.023751	-0.503497	-0.204891
57	1	-3.060913	3.938877	-0.369930
58	7	-1.311317	2.859946	-0.150467
59	8	6.802894	-6.248378	2.414209
60	6	6.417391	-5.202778	1.925432
61	6	5.073712	-5.166234	1.164973
62	8	6.998091	-4.034584	1.996786
63	7	5.064507	-4.207963	0.023245
64	1	4.321270	-4.841625	1.892355
65	1	4.804134	-6.179302	0.840944
66	6	5.610326	-4.869691	-1.192813
67	6	3.689042	-3.719223	-0.222042
68	8	6.684346	0.004105	0.963541
69	8	9.007425	-2.033530	0.696757
70	8	6.576553	-1.697661	3.009134

71	6	7.118046	-5.133662	-1.133742
72	1	5.384650	-4.237274	-2.056600
73	1	5.094202	-5.828551	-1.361914
74	6	3.623581	-2.445945	-1.068222
75	1	3.236184	-3.527949	0.755852
76	1	3.067396	-4.491962	-0.705134
77	6	6.956740	0.879422	0.048148
78	6	9.886005	-2.838100	0.133355
79	7	7.910239	-3.879399	-1.034081
80	1	7.403241	-5.708877	-2.027610
81	1	7.355653	-5.762685	-0.274245
82	7	4.419727	-1.331875	-0.512217
83	1	3.999541	-2.651817	-2.073486
84	1	2.564559	-2.163764	-1.199188
85	6	7.790060	0.327627	-1.124867
86	8	6.569339	2.051815	0.040963
87	6	9.255859	-4.128919	-0.432433
88	8	11.080992	-2.642194	0.043607
89	6	8.046495	-3.251081	-2.376968
90	6	4.820469	-0.387704	-1.584895
91	6	3.767514	-0.676418	0.667648
92	7	7.277395	-1.000625	-1.569296
93	1	7.804616	1.049908	-1.951635
94	1	8.810279	0.183244	-0.758786
95	1	9.938279	-4.589818	-1.156665
96	1	9.127784	-4.814001	0.411370
97	6	8.313405	-1.743933	-2.338231
98	1	8.860372	-3.733544	-2.938504
99	1	7.129310	-3.449007	-2.939533
100	6	6.047199	-0.851449	-2.377777
101	1	5.028699	0.586496	-1.149691
102	1	3.993833	-0.237585	-2.298716
103	1	3.180818	-1.441265	1.183980
104	1	4.566743	-0.354150	1.338096
105	6	2.889807	0.545017	0.423636
106	1	8.373423	-1.372809	-3.373501
107	1	9.280875	-1.547422	-1.876260
108	1	6.211929	-0.127902	-3.193846
109	1	5.836136	-1.812684	-2.855119
110	6	1.507037	0.467133	0.225035
111	6	3.461337	1.827014	0.476757
112	6	0.733643	1.626814	0.091943
113	1	1.023707	-0.503522	0.204838
114	6	2.644399	2.939458	0.328791
115	1	4.534411	1.970203	0.625742
116	7	1.311349	2.859915	0.150445
117	1	3.060968	3.938805	0.369927
118	44	0.000034	4.508794	0.000003
119	1	-0.890292	3.226501	-2.723211
120	6	-0.120341	3.920248	-3.039368
121	6	0.228407	4.047673	-4.379527
122	6	1.431390	5.540260	-2.391569
123	6	1.224598	4.959526	-4.727277
124	1	-0.274966	3.444516	-5.127355
125	6	2.003616	6.305575	-1.264734
126	6	1.828859	5.709664	-3.722400
127	1	1.525731	5.088388	-5.761958
128	6	3.006606	7.269269	-1.414271
129	1	2.602673	6.423259	-3.977509
130	6	1.954643	6.681858	1.037899
131	6	3.487543	7.947971	-0.297928

132	1	3.414893	7.490957	-2.392720
133	6	2.949484	7.650115	0.953372
134	1	1.511049	6.415715	1.989824
135	1	4.267875	8.694403	-0.405481
136	1	3.291000	8.152547	1.851816
137	7	0.458693	4.643420	-2.061414
138	7	1.488448	6.016287	-0.036064
139	1	0.890331	3.226436	2.723195
140	6	0.120397	3.920195	3.039363
141	6	-0.228348	4.047606	4.379524
142	6	-1.224519	4.959475	4.727290
143	1	0.275011	3.444426	5.127343
144	6	-1.431299	5.540251	2.391592
145	6	-1.828764	5.709643	3.722425
146	1	-1.525649	5.088326	5.761973
147	6	-2.003509	6.305597	1.264769
148	1	-2.602562	6.423250	3.977546
149	6	-3.006479	7.269309	1.414323
150	6	-3.487403	7.948040	0.297990
151	1	-3.414763	7.490990	2.392775
152	6	-1.954527	6.681918	-1.037857
153	6	-2.949348	7.650194	-0.953314
154	1	-4.267719	8.694486	0.405556
155	1	-1.510938	6.415781	-1.989787
156	1	-3.290854	8.152648	-1.851750
157	7	-0.458622	4.643396	2.061421
158	7	-1.488347	6.016319	0.036095
159	8	-6.576588	-1.697741	-3.009166
160	1	-6.985435	-2.480135	-3.428814
161	1	-7.085373	-0.904622	-3.250324
162	1	6.985425	-2.480006	3.428846
163	1	7.085308	-0.904504	3.250231
164	70	-6.879133	-2.248203	-0.677968
165	70	6.879103	-2.248219	0.677964

E(RB+HF-LYP) = -4323.5225321 Hartree

[Yb₂.1.Ru(Bpy)₂]²⁺·2H₂O [$\Delta(\delta\delta\delta\delta)$] HF/3-21G (0 Imaginary Frequencies)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	4.057781	-1.531113	-0.248945
2	6	4.264161	-0.856209	-1.559003
3	6	5.482815	0.056152	-1.593504
4	7	6.742665	-0.683740	-1.281380
5	6	7.295803	-1.295183	-2.523004
6	6	8.255872	-2.443047	-2.232277
7	7	7.632898	-3.503432	-1.381706
8	6	6.717189	-4.366373	-2.174768
9	6	5.802398	-5.207133	-1.285283
10	7	4.897709	-4.389906	-0.415031
11	6	3.720599	-3.861398	-1.142256
12	6	3.107432	-2.670741	-0.391275
13	6	7.706106	0.257728	-0.603797
14	6	6.990247	0.678149	0.683573
15	8	6.678104	1.845954	0.887635
16	8	6.613618	-0.339627	1.399949
17	6	8.734822	-4.279075	-0.725877
18	6	9.448331	-3.376012	0.302721

19	8	10.589668	-3.594383	0.618677
20	8	8.664128	-2.415564	0.751032
21	6	4.483751	-5.213097	0.767590
22	6	5.427969	-4.893526	1.925783
23	8	5.005385	-4.887240	3.078717
24	8	6.594831	-4.484024	1.540843
25	1	7.905177	1.120318	-1.225966
26	1	8.612636	-0.273913	-0.363863
27	1	9.447516	-4.641072	-1.457308
28	1	8.317314	-5.112726	-0.183508
29	1	3.479713	-4.967964	1.074203
30	1	4.505953	-6.271322	0.527971
31	6	3.698005	-0.606133	0.884569
32	1	3.213611	-1.204046	1.642206
33	1	4.616158	-0.249031	1.308583
34	6	2.832500	0.613225	0.581200
35	6	1.475451	0.539465	0.291722
36	6	3.406194	1.872415	0.704697
37	6	0.730480	1.695143	0.140567
38	6	2.614426	2.985667	0.528904
39	1	4.448926	1.987609	0.940093
40	1	1.006133	-0.416287	0.212168
41	1	3.025225	3.967155	0.615898
42	7	1.310123	2.901718	0.259858
43	8	-5.004242	-4.886377	-3.078385
44	6	-5.427325	-4.893396	-1.925596
45	6	-4.483550	-5.213368	-0.767202
46	8	-6.594422	-4.484344	-1.540918
47	7	-4.897702	-4.390043	0.415299
48	1	-3.479323	-4.968558	-1.073447
49	1	-4.506215	-6.271579	-0.527590
50	6	-5.802427	-5.207180	1.285605
51	6	-3.720704	-3.861325	1.142551
52	8	-6.613712	-0.339741	-1.400227
53	8	-8.664035	-2.415987	-0.751230
54	8	-5.536764	-2.279433	-2.747237
55	6	-6.717261	-4.366326	2.174952
56	6	-3.107538	-2.670709	0.391492
57	6	-6.990296	0.678036	-0.683844
58	6	-9.448232	-3.376436	-0.302886
59	7	-7.632928	-3.503497	1.381727
60	7	-4.057895	-1.531093	0.249032
61	6	-7.706255	0.257645	0.603459
62	8	-6.678052	1.845835	-0.887839
63	6	-8.734746	-4.279284	0.725906
64	8	-10.589475	-3.594989	-0.619027
65	6	-8.256017	-2.443034	2.232106
66	6	-4.264339	-0.856041	1.559011
67	6	-3.698035	-0.606177	-0.884518
68	7	-6.742802	-0.683758	1.281137
69	1	-7.905411	1.120236	1.225596
70	1	-8.612740	-0.274053	0.363480
71	1	-9.447471	-4.641253	1.457323
72	1	-8.317139	-5.112986	0.183682
73	6	-7.296017	-1.295115	2.522796
74	6	-5.483039	0.056264	1.593334
75	1	-3.213600	-1.204139	-1.642081
76	1	-4.616164	-0.249107	-1.308606
77	6	-2.832570	0.613194	-0.581124
78	6	-1.475530	0.539449	-0.291615
79	6	-3.406272	1.872380	-0.704656

80	6	-0.730572	1.695137	-0.140457
81	1	-1.006205	-0.416299	-0.212049
82	6	-2.614523	2.985640	-0.528839
83	1	-4.448996	1.987554	-0.940101
84	7	-1.310222	2.901703	-0.259762
85	1	-3.025328	3.967125	-0.615835
86	44	-0.000057	4.599590	0.000038
87	1	0.587298	3.324592	2.826974
88	6	-0.183518	4.023251	3.065747
89	6	-0.652340	4.158560	4.355123
90	6	-1.628540	5.659600	2.277492
91	6	-1.650925	5.082868	4.596872
92	1	-0.243753	3.560308	5.141752
93	6	-2.093784	6.437146	1.099937
94	6	-2.144191	5.838943	3.548687
95	1	-2.041265	5.218357	5.584684
96	6	-3.067273	7.415572	1.182115
97	1	-2.915485	6.553153	3.731438
98	6	-1.876791	6.805275	-1.180151
99	6	-3.446326	8.097481	0.039108
100	1	-3.530501	7.652328	2.113650
101	6	-2.842404	7.789568	-1.164482
102	1	-1.381815	6.531446	-2.085160
103	1	-4.201013	8.854977	0.092672
104	1	-3.110467	8.294756	-2.068006
105	7	-0.659123	4.756462	2.056351
106	7	-1.515242	6.146223	-0.077163
107	1	-0.587420	3.324525	-2.826871
108	6	0.183405	4.023169	-3.065659
109	6	0.652239	4.158434	-4.355035
110	6	1.650835	5.082725	-4.596804
111	1	0.243653	3.560161	-5.141649
112	6	1.628431	5.659533	-2.277443
113	6	2.144096	5.838831	-3.548639
114	1	2.041185	5.218179	-5.584616
115	6	2.093668	6.437117	-1.099911
116	1	2.915397	6.553028	-3.731406
117	6	3.067154	7.415544	-1.182116
118	6	3.446201	8.097491	-0.039131
119	1	3.530385	7.652271	-2.113657
120	6	1.876665	6.805321	1.180164
121	6	2.842275	7.789616	1.164468
122	1	4.200887	8.854987	-0.092716
123	1	1.381685	6.531521	2.085181
124	1	3.110333	8.294834	2.067976
125	7	0.659007	4.756407	-2.056281
126	7	1.515121	6.146232	0.077197
127	8	5.537139	-2.279501	2.747433
128	1	5.449024	-3.082660	3.304693
129	1	5.900089	-1.506246	3.201243
130	1	-5.448275	-3.082603	-3.304466
131	1	-5.899713	-1.506201	-3.201077
132	70	6.530062	-2.444599	0.616308
133	70	-6.530020	-2.444722	-0.616431
134	1	2.201100	-2.359743	-0.909574
135	1	2.833514	-2.988549	0.604073
136	1	2.959700	-4.629812	-1.260357
137	1	4.027700	-3.568236	-2.133790
138	1	5.209470	-5.872074	-1.909912
139	1	6.401889	-5.815181	-0.630801
140	1	6.124257	-3.732818	-2.819693

141	1	7.290055	-5.032716	-2.815501
142	1	8.596423	-2.872883	-3.171245
143	1	9.123295	-2.067642	-1.715459
144	1	6.462580	-1.653428	-3.111411
145	1	7.807244	-0.539905	-3.114785
146	1	5.554282	0.507190	-2.580646
147	1	5.373935	0.864911	-0.893717
148	1	4.383931	-1.623171	-2.306975
149	1	3.381700	-0.281274	-1.830206
150	1	-5.209519	-5.872032	1.910353
151	1	-6.401915	-5.815339	0.631219
152	1	-7.290155	-5.032611	2.815722
153	1	-6.124371	-3.732703	2.819844
154	1	-9.123393	-2.067719	1.715148
155	1	-8.596664	-2.872764	3.171090
156	1	-6.462814	-1.653271	3.111281
157	1	-7.807509	-0.539786	3.114461
158	1	-5.554645	0.507348	2.580442
159	1	-5.374179	0.864983	0.893498
160	1	-4.384110	-1.622910	2.307073
161	1	-3.381906	-0.281040	1.830160
162	1	-2.833583	-2.988603	-0.603819
163	1	-2.201230	-2.359657	0.909798
164	1	-4.027932	-3.568063	2.134013
165	1	-2.959756	-4.629661	1.260834

E(RB+HF-LYP) = -4274.2647969 Hartree
Zero-point correction = 1.449461 Hartree/particle
Sum of electronic and thermal Energies = -4272.738866 Hartree
Sum of electronic and thermal Enthalpies = -4272.737922 Hartree
Sum of electronic and thermal Free Energies = -4272.931088 Hartree

[Yb₂.1.Ru(Bpy)₂]²⁺·2H₂O [Δ(δδδδ)] B3LYP/6-31G(d)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-4.042985	-1.513599	0.327696
2	6	-4.252849	-0.945246	1.674794
3	6	-5.513499	-0.099705	1.810987
4	7	-6.757456	-0.834342	1.468673
5	6	-7.258977	-1.568660	2.654959
6	6	-8.176098	-2.735380	2.300056
7	7	-7.560513	-3.707679	1.355704
8	6	-6.588668	-4.587092	2.049496
9	6	-5.641179	-5.317100	1.096590
10	7	-4.787198	-4.423432	0.271340
11	6	-3.626408	-3.902440	1.011011
12	6	-3.061106	-2.619711	0.378957
13	6	-7.747882	0.142419	0.917851
14	6	-7.133048	0.679740	-0.392969
15	8	-6.866901	1.875385	-0.518578
16	8	-6.816381	-0.260000	-1.232068
17	6	-8.660758	-4.482822	0.710262
18	6	-9.455361	-3.595088	-0.278646
19	8	-10.608790	-3.858994	-0.537112
20	8	-8.745098	-2.595913	-0.769074
21	6	-4.363447	-5.128292	-0.974359
22	6	-5.258051	-4.677994	-2.141012
23	8	-4.770581	-4.516457	-3.264430

24	8	-6.462918	-4.373450	-1.785233
25	1	-7.934409	0.962463	1.623429
26	1	-8.684791	-0.379003	0.703928
27	1	-9.342250	-4.907799	1.458259
28	1	-8.230669	-5.306169	0.133743
29	1	-3.328033	-4.883100	-1.219221
30	1	-4.409090	-6.218131	-0.846075
31	6	-3.768783	-0.504317	-0.736641
32	1	-3.354300	-1.048319	-1.589730
33	1	-4.727312	-0.111933	-1.078487
34	6	-2.883083	0.698865	-0.438589
35	6	-1.500314	0.625447	-0.233940
36	6	-3.458090	1.979038	-0.475037
37	6	-0.733917	1.786833	-0.091150
38	6	-2.647651	3.096457	-0.320444
39	1	-4.527938	2.107262	-0.644741
40	1	-1.012835	-0.342684	-0.223381
41	1	-3.066769	4.095057	-0.356695
42	7	-1.314777	3.019730	-0.142621
43	8	4.770399	-4.516159	3.264506
44	6	5.257895	-4.677754	2.141107
45	6	4.363317	-5.128117	0.974462
46	8	6.462785	-4.373288	1.785346
47	7	4.787129	-4.423353	-0.271269
48	1	3.327901	-4.882890	1.219278
49	1	4.408953	-6.217964	0.846255
50	6	5.641061	-5.317121	-1.096465
51	6	3.626386	-3.902313	-1.010982
52	8	6.816587	-0.259902	1.231915
53	8	8.745086	-2.595996	0.769103
54	8	5.549884	-1.976212	2.814421
55	6	6.588612	-4.587221	-2.049387
56	6	3.061145	-2.619530	-0.378979
57	6	7.133429	0.679750	0.392785
58	6	9.455293	-3.595263	0.278785
59	7	7.560486	-3.707819	-1.355626
60	7	4.043092	-1.513483	-0.327701
61	6	7.748181	0.142264	-0.917998
62	8	6.867298	1.875414	0.518242
63	6	8.660673	-4.482986	-0.710116
64	8	10.608716	-3.859190	0.537249
65	6	8.176140	-2.735630	-2.300043
66	6	4.253027	-0.945155	-1.674801
67	6	3.768925	-0.504175	0.736617
68	7	6.757657	-0.834450	-1.468728
69	1	7.934785	0.962224	-1.623654
70	1	8.685046	-0.379225	-0.704032
71	1	9.342163	-4.908034	-1.458074
72	1	8.230521	-5.306279	-0.133568
73	6	7.259099	-1.568860	-2.654993
74	6	5.513747	-0.099719	-1.811028
75	1	3.354484	-1.048162	1.589729
76	1	4.727465	-0.111764	1.078409
77	6	2.883175	0.698984	0.438566
78	6	1.500402	0.625510	0.233965
79	6	3.458127	1.979179	0.474978
80	6	0.733956	1.786866	0.091165
81	1	1.012959	-0.342639	0.223441
82	6	2.647645	3.096565	0.320397
83	1	4.527963	2.107449	0.644684
84	7	1.314767	3.019784	0.142610

85	1	3.066724	4.095182	0.356639
86	44	-0.000037	4.669045	0.000002
87	1	-0.911539	3.380926	-2.715665
88	6	-0.150446	4.080977	-3.039143
89	6	0.179550	4.214630	-4.383495
90	6	1.398308	5.709908	-2.407089
91	6	1.164039	5.135029	-4.741823
92	1	-0.329468	3.609893	-5.126218
93	6	1.981710	6.474733	-1.285578
94	6	1.776397	5.886356	-3.742664
95	1	1.449875	5.269514	-5.780121
96	6	2.976373	7.445405	-1.445736
97	1	2.541159	6.606711	-4.006046
98	6	1.965727	6.840352	1.019456
99	6	3.470293	8.121930	-0.333692
100	1	3.367684	7.674671	-2.429379
101	6	2.953860	7.814499	0.924425
102	1	1.538005	6.567609	1.976760
103	1	4.243879	8.874117	-0.449702
104	1	3.306451	8.314437	1.819984
105	7	0.436094	4.805531	-2.066561
106	7	1.486595	6.177340	-0.050547
107	1	0.911499	3.380929	2.715652
108	6	0.150390	4.080959	3.039138
109	6	-0.179606	4.214593	4.383492
110	6	-1.164116	5.134965	4.741830
111	1	0.329431	3.609864	5.126209
112	6	-1.398410	5.709851	2.407101
113	6	-1.776498	5.886283	3.742677
114	1	-1.449949	5.269439	5.780129
115	6	-1.981840	6.474662	1.285596
116	1	-2.541276	6.606617	4.006068
117	6	-2.976533	7.445302	1.445761
118	6	-3.470483	8.121812	0.333721
119	1	-3.367846	7.674554	2.429407
120	6	-1.965880	6.840288	-1.019437
121	6	-2.954046	7.814402	-0.924400
122	1	-4.244093	8.873973	0.449738
123	1	-1.538152	6.567565	-1.976743
124	1	-3.306658	8.314330	-1.819955
125	7	-0.436172	4.805505	2.066565
126	7	-1.486721	6.177290	0.050560
127	8	-5.549900	-1.976533	-2.814515
128	1	-5.443270	-2.790590	-3.370801
129	1	-6.074448	-1.312585	-3.292401
130	1	5.443214	-2.790209	3.370789
131	1	6.074430	-1.312228	3.292262
132	70	-6.619498	-2.443789	-0.667226
133	70	6.619507	-2.443712	0.667206
134	1	-2.151943	-2.334710	0.938054
135	1	-2.753093	-2.836452	-0.648424
136	1	-2.812636	-4.644214	1.068362
137	1	-3.930713	-3.712443	2.043961
138	1	-5.021378	-6.014839	1.683191
139	1	-6.226947	-5.921070	0.402730
140	1	-6.013036	-3.973959	2.750805
141	1	-7.114668	-5.339057	2.658523
142	1	-8.485282	-3.241791	3.227457
143	1	-9.086937	-2.354868	1.833812
144	1	-6.388002	-1.936356	3.207212
145	1	-7.794180	-0.889114	3.336567

146	1	-5.564106	0.284188	2.842007
147	1	-5.446465	0.779476	1.169724
148	1	-4.303449	-1.779257	2.378164
149	1	-3.388217	-0.335177	1.988521
150	1	5.021223	-6.014845	-1.683044
151	1	6.226775	-5.921105	-0.402568
152	1	7.114586	-5.339253	-2.658357
153	1	6.013027	-3.974102	-2.750748
154	1	9.087020	-2.355165	-1.833838
155	1	8.485264	-3.242120	-3.227421
156	1	6.388087	-1.936517	-3.207211
157	1	7.794342	-0.889380	-3.336635
158	1	5.564337	0.284130	-2.842063
159	1	5.446831	0.779485	-1.169784
160	1	4.303573	-1.779176	-2.378164
161	1	3.388457	-0.335016	-1.988551
162	1	2.753066	-2.836221	0.648393
163	1	2.152025	-2.334476	-0.938122
164	1	3.930727	-3.712350	-2.043926
165	1	2.812579	-4.644050	-1.068333

E (RB+HF-LYP) = -4323.5104974 Hartree