

Table SI-1. Values of the intersystem crossing rate, k_{23} , and triplet relaxation rate, k_{31} , of Rhodamine 6G in different solvents.

Solvent	k_{23} (s^{-1})	k_{31} (s^{-1})	Reference
Water	$(1.1\pm 0.2) 10^6$	$(0.49\pm 0.5) 10^6$	(a) Widengren 1995
	$(4\pm 1) 10^5$	$(4\pm 1) 10^1$	(b) Korobov 1978 (77K)
	$7.3 10^5$	$3.9 10^5$	(k) Eggeling 1998
	$8.8 10^5$	$5.3 10^5$	(l) Heupel 1997
	$1.1 10^6$	$5.0 10^5$	(m) Chmyrov 2008
Methanol	$(3.0\pm 0.6) 10^6$	$(3.5\pm 0.4) 10^6$	(a) Widengren 1995
Ethanol	$(2.0\pm 0.4) 10^6$	$(2.9\pm 0.3) 10^6$	(a) Widengren 1995
	$(4.2\pm 0.4) 10^5$	10^3-10^4	(c) Dempster 1973 (excitation dependent)
	$5.3 10^5$	$2.5 10^5$	(d) Asimov 1990
	$(3.4\pm 1.4) 10^6$	$4 10^6$	(e) Webb 1970
	$1.1 10^5$	0.59	(i) Yamashita 1974, 1975, 1977 (ESR, 77K)
	$2.3 10^6$	$2.6 10^6$	(l) Heupel 1997
Rh6G ethanol-methanol 4:1		0.87	(j) Antonucci 1973 (ESR, 77K)
RhB ethanol-methanol 4:1		1.4	(j) Antonucci 1973 (ESR, 77K)
Propanol	$2.5\pm 0.5 10^6$	$2.5\pm 0.5 10^6$	(a) Widengren 1995
Ethylene glycol	$(3.5\pm 0.7) 10^5$	$(2.0\pm 0.2) 10^5$	(a) Widengren 1995
	$6.4 10^5$	$(1.1-2.5) 10^5$	(f) Thiel 1992 (solution dependent)
	$6.4 10^6$	$8.0 10^6$	(g) Teschke 1975
	$3.8 10^5$	$1.3 10^5$	(d) Asimov 1990
	$8.3 10^5$	$2.2 10^5$	(l) Heupel 1997
	$7.7 10^5$	10^4	(n) Heupel 1999 ($[O_2] < 0.01\text{mM}$)
	$1.35 10^6$	$9.3 10^5$	(n) Heupel 1999 ($[O_2] = 0.58\text{mM}$)
Acetonitrile	$2.7 10^6$	$2 10^6$	(h) Stracke 1999

(a) Widengren, J. and Metz, U. and Rigler, R. Journal of Physical Chemistry **1995**, 99, 13368-13379

(b) Korobov, V.E. and Chibisov, A.K. Journal of Photochemistry **1978**, 9, 411-424

(c) Dempster, D.N. and Morrow, T. and Quinn, M.F. Journal of Photochemistry, **1973/4** 343-359

(d) Asimov, M.M. and Gavrilenko, V.N. and Rubinov, A.N. Journal of Luminescence **1990**, 46, 243-249

(e) Webb, J.P. and McColgin, W.C. and Peterson, O.G. and Stockman, D.L. and Eberly, J.H. Journal of Chemical Physics **1970**, 53, 4227-4229

(f) Thiel, E. and Drexhage, K.H. Chemical Physics Letters **1992**, 3-4, 329-334

(g) Teschke, O. and Dienes, A. and Holtom, G. Optics Communications **1975**, 13, 318-320

(h) Stracke, F. and Heupel, M. and Thiel, E. Journal of Photochemistry and Photobiology A, **1999**, 126, 51-58

(i) Yamashita, M. and Ikeda, H. and Kashiwagi, H. Journal of Physical Chemistry **1975**, 63, 1127-1132; Yamashita, M. and Kashiwagi, H. Journal of Physical Chemistry **1974**, 78, 2006-2009; Yamashita, M. and Kuniyasu, A. and Kashiwagi, H. Journal of Chemical Physics **1977**, 66, 986-988

(j) Antonucci, F.R. and Tolley, L.G. Journal of Physical Chemistry **1973**, 77, 2712

(k) Eggeling, C. and Widengren, J. and Rigler, R. and Seidel, C.A.M Analytical Chemistry **1998**, 70, 2651-2659

(l) Heupel, M. and Thiel, E. Journal of Fluorescence **1997**, 7, 371-375

(m) Chmyrov, A. and Arden-Jacob, J. and Zilles, A. and Drexhage, K.H. and Widengren, J. Photochemical and Photobiological Sciences **2008**, 7, 1378-1385

(n) Heupel, M. and Gregor, I. and Becker, S. and Thiel, E. International journal of photoenergy, **1999**, 1, 165-172.

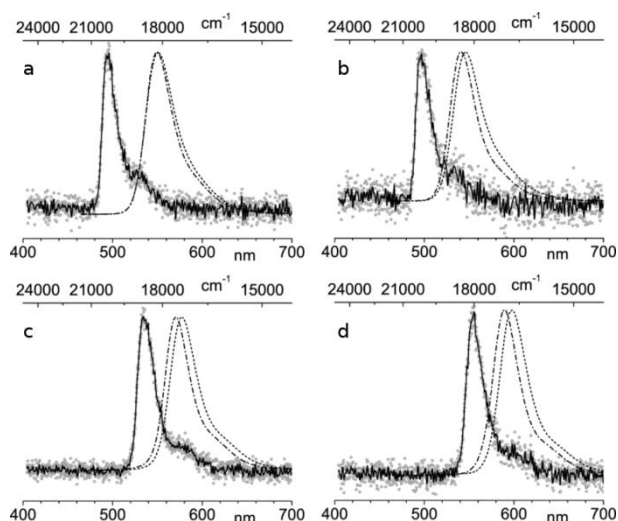


Figure SI-1. Comparison of gas phase (solid line) dispersed fluorescence measurements ($T = 85$ K) of rhodamine (a) Rh6G^+ , (b) Rh575^+ , (c) RhB^+ and (d) Rh101^+ with the corresponding solution spectra (water – dotted, and methanol dashed-dotted line, at $T = 293$ K) at 10^{-4}M and an excitation wavelength of 488nm.

Table SI-2. Maxima of the fluorescence emission spectra in solution at 293K and concentrations $\sim 10^{-4}\text{M}$.

	Solution (exp.)	
	S_1-S_0 (H_2O)	S_1-S_0 (MeOH)
Rh6G^+	2.25	2.25
Rh575^+	2.27	2.29
RhB^+	2.15	2.17
Rh101^+	2.07	2.10

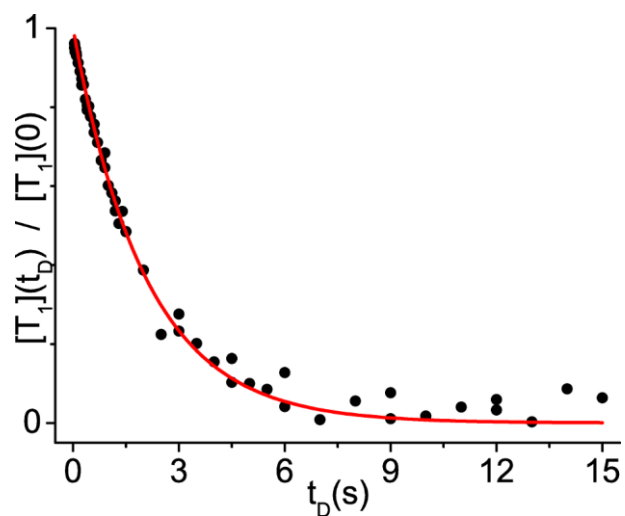


Figure SI-2. Example of Rh6G⁺ triplet state populations at room temperature (T=286K) as a function of the time delay t_D . The corresponding lifetime is 2060 ms.

Table SI-3. XYZ files.

Table 1: B3LYP/def2-SVP optimized S0 geometry of Rh6G⁺ in Å.

C	-0.2234095	-3.5216863	0.4939399
C	-0.0509814	-2.6712461	-0.6237775
C	0.1044195	-3.2426319	-1.8963618
C	0.0902808	-4.6300222	-2.0664754
C	-0.0800638	-5.4682830	-0.9617488
C	-0.2355809	-4.9140666	0.3088648
C	-0.0249629	-1.1779906	-0.5210552
C	-1.2114238	-0.4273212	-0.6878380
C	-1.1428653	0.9949651	-0.6436075
O	0.0416739	1.6218009	-0.4610482
C	1.1971100	0.9323917	-0.3229202
C	1.2004528	-0.4917967	-0.3580941
C	-2.5059460	-0.9985240	-0.8828740
C	-3.6444448	-0.2418202	-1.0252316
C	-3.5326864	1.2034537	-0.9754176
C	-2.2654333	1.7960729	-0.7842094
C	2.4680780	-1.1314816	-0.2032390
C	3.6409196	-0.4365928	-0.0283243
C	3.5956069	1.0128407	0.0018957
C	2.3564734	1.6724552	-0.1500869
C	-4.9936430	-0.8804280	-1.2290081
N	-4.6449886	1.9588825	-1.1141892
C	-4.6893402	3.4156618	-1.0849036
C	-6.1138694	3.9219084	-1.2727302
N	4.7421454	1.7078096	0.1740023
C	4.8530046	3.1603877	0.2261994
C	6.2998248	3.5899273	0.4335964
C	4.9599747	-1.1464878	0.1322939
C	-0.3911335	-2.9254936	1.8590290
O	-0.5408840	-3.8493189	2.8111220
C	-0.7107929	-3.3810435	4.1685554
C	-0.8570032	-4.5893394	5.0679398
O	-0.3908449	-1.7316680	2.0755444
H	-2.5867271	-2.0865086	-0.9186452
H	-2.1381752	2.8762164	-0.7399893
H	2.2787408	2.7580472	-0.1332237
H	2.4985505	-2.2224027	-0.2253026
H	5.6002393	1.1803442	0.2779891
H	0.2380424	-2.5907093	-2.7633477
H	0.2129681	-5.0534620	-3.0665179
H	-0.0918999	-6.5532728	-1.0893504
H	-0.3694355	-5.5557610	1.1802896
H	5.6749341	-0.8659127	-0.6618433
H	4.8306634	-2.2363249	0.0861535
H	5.4347972	-0.9120526	1.1018554
H	-5.4531881	-0.5701450	-2.1845923
H	-5.6985348	-0.6129421	-0.4214734
H	-4.9142676	-1.9758885	-1.2446064
H	4.2199011	3.5482738	1.0451805
H	4.4585868	3.5932369	-0.7114499
H	6.7022851	3.1974275	1.3816829
H	6.3682500	4.6869060	0.4705614
H	6.9432286	3.2421150	-0.3910168
H	-4.0345627	3.8195063	-1.8787928
H	-4.2810441	3.7767705	-0.1231888
H	-6.5284606	3.6016981	-2.2425539
H	-6.1319417	5.0212132	-1.2485401
H	-6.7771936	3.5586955	-0.4708508
H	-1.5953646	-2.7248333	4.2027434
H	0.1618792	-2.7638341	4.4361712
H	-1.7339988	-5.1916900	4.7847920
H	-0.9883011	-4.2614150	6.1108045
H	0.0364987	-5.2308653	5.0200400
H	-5.5261554	1.4779262	-1.2468057

Table 2: B3LYP/def2-SVP optimized S1 geometry of Rh6G⁺ in Å.

C	-0.0962023	-3.5672789	0.5311178
C	-0.3681284	-2.6923112	-0.5625393
C	-0.6939864	-3.2754218	-1.8070215
C	-0.7117860	-4.6577444	-1.9852267
C	-0.4154056	-5.5073352	-0.9118118
C	-0.1204121	-4.9598133	0.3345556
C	-0.2999063	-1.2216044	-0.4773050
C	-1.4181688	-0.4030617	-0.7515721
C	-1.2969031	1.0299251	-0.7249506
O	-0.1105239	1.6272842	-0.4354346
C	0.9938567	0.8753255	-0.1998932
C	0.9728447	-0.5258176	-0.2097966
C	-2.7399937	-0.9002972	-1.0044849
C	-3.8256656	-0.0896344	-1.2545317
C	-3.6434355	1.3486756	-1.2534703
C	-2.3647828	1.8765045	-0.9720436
C	2.2198174	-1.1802846	-0.0130273
C	3.4155119	-0.5181902	0.2121532
C	3.3948442	0.9172290	0.2471222
C	2.1712316	1.6016548	0.0283139
C	-5.1906203	-0.6713079	-1.5097952
N	-4.7028442	2.1574001	-1.5049048
C	-4.6718380	3.6118484	-1.5209255
C	-6.0453874	4.1861971	-1.8441344
N	4.5407064	1.6134773	0.4804921
C	4.6780497	3.0598768	0.5485960
C	6.1194521	3.4633733	0.8314931
C	4.7079149	-1.2640403	0.4204307
C	0.1166630	-3.0075715	1.8961855
O	0.2274375	-3.9514389	2.8396724
C	0.4071094	-3.5099349	4.2020255
C	0.5018999	-4.7362131	5.0844115
O	0.1748979	-1.8172229	2.1456587
H	-2.8901290	-1.9802789	-0.9845372
H	-2.1857001	2.9498957	-0.9339157
H	2.1118928	2.6890920	0.0217390
H	2.2328701	-2.2710998	-0.0478089
H	5.3848137	1.0690675	0.6289965
H	-0.8972052	-2.6202250	-2.6575545
H	-0.9447291	-5.0735718	-2.9688740
H	-0.4232394	-6.5914911	-1.0457833
H	0.0825008	-5.6093791	1.1866065
H	5.4683089	-0.9961875	-0.3357200
H	4.5506075	-2.3490019	0.3492635
H	5.1453301	-1.0645492	1.4159120
H	-5.5740836	-0.3919190	-2.5079149
H	-5.9289797	-0.3242337	-0.7646952
H	-5.1683224	-1.7684980	-1.4633885
H	4.0075679	3.4548007	1.3353520
H	4.3357234	3.5054841	-0.4048118
H	6.4660750	3.0604942	1.7968521
H	6.2012037	4.5589813	0.8782118
H	6.7975506	3.1105960	0.0376882
H	-3.9301049	3.9563794	-2.2660426
H	-4.3249271	3.9845392	-0.5385732
H	-6.3937147	3.8563529	-2.8364698
H	-6.0048231	5.2851734	-1.8523985
H	-6.7925225	3.8844775	-1.0920218
H	-0.4427772	-2.8644227	4.4766498
H	1.3155933	-2.8877923	4.2535169
H	-0.4149175	-5.3423771	5.0202547
H	0.6382766	-4.4300339	6.1332639
H	1.3568667	-5.3676357	4.7968283
H	-5.5952707	1.7167878	-1.6939697

Table 3: B3LYP/def2-SVP optimized T1 geometry of Rh6G⁺ in Å.

C	-0.1274734	-3.5258519	0.4957058
C	-0.1158908	-2.6864830	-0.6495898
C	-0.1610624	-3.2912773	-1.9185220
C	-0.2036753	-4.6799760	-2.0660797
C	-0.2091548	-5.4994573	-0.9346051
C	-0.1768228	-4.9220385	0.3342017
C	-0.0748897	-1.1969069	-0.5802990
C	-1.2560740	-0.4219737	-0.7488118
C	-1.1839076	1.0080805	-0.6999824
O	0.0070472	1.6465446	-0.4951705
C	1.1564331	0.9367251	-0.3252072
C	1.1558798	-0.4947277	-0.3651450
C	-2.5557265	-0.9749542	-0.9518484
C	-3.6965999	-0.2068696	-1.1085414
C	-3.5744914	1.2273348	-1.0618602
C	-2.2933454	1.8095388	-0.8519276
C	2.4125456	-1.1332315	-0.1905337
C	3.5958674	-0.4428926	0.0194026
C	3.5510350	0.9978157	0.0609179
C	2.3079658	1.6649285	-0.1192756
C	-5.0432526	-0.8480643	-1.3194775
N	-4.6785591	2.0058033	-1.2137216
C	-4.7132082	3.4620756	-1.1850193
C	-6.1305376	3.9806820	-1.3922112
N	4.6949799	1.6995092	0.2699571
C	4.8158182	3.1505737	0.3424804
C	6.2586888	3.5696861	0.5925305
C	4.8999579	-1.1720877	0.2041822
C	-0.1011539	-2.9367235	1.8757190
O	-0.3425580	-3.8527834	2.8242466
C	-0.3269290	-3.4021694	4.1945740
C	-0.6185287	-4.5915943	5.0846226
O	0.1142011	-1.7699168	2.1263809
H	-2.6474920	-2.0616558	-0.9823579
H	-2.1589845	2.8891334	-0.8020967
H	2.2342062	2.7511761	-0.0976655
H	2.4392430	-2.2233329	-0.2211222
H	5.5496166	1.1659229	0.3924529
H	-0.1563749	-2.6525457	-2.8056447
H	-0.2304958	-5.1197923	-3.0664474
H	-0.2412801	-6.5866457	-1.0391480
H	-0.1905480	-5.5511483	1.2244971
H	5.6404665	-0.8938977	-0.5670737
H	4.7544013	-2.2585290	0.1384561
H	5.3516183	-0.9618123	1.1902911
H	-5.4953099	-0.5476102	-2.2818453
H	-5.7563627	-0.5782005	-0.5199185
H	-4.9607884	-1.9431959	-1.3264265
H	4.1599676	3.5275672	1.1479381
H	4.4447737	3.5913645	-0.6004635
H	6.6343274	3.1665276	1.5469211
H	6.3282713	4.6659060	0.6434479
H	6.9221333	3.2302459	-0.2193590
H	-4.0425212	3.8583118	-1.9691698
H	-4.3133532	3.8175125	-0.2177884
H	-6.5344862	3.6653565	-2.3679839
H	-6.1376327	5.0800357	-1.3676270
H	-6.8080096	3.6241786	-0.5993321
H	-1.0765738	-2.6025901	4.3098471
H	0.6574383	-2.9539747	4.4070720
H	-1.6047423	-5.0248497	4.8567639
H	-0.6171031	-4.2763837	6.1396761
H	0.1429280	-5.3771479	4.9602287
H	-5.5639301	1.5324277	-1.3571997

Table 4: B3LYP/def2-SVP optimized S0 geometry of Rh575⁺ in Å.

C	0.0002452	-0.8960768	0.1596282
C	-1.2041824	-0.1515119	0.2703223
C	1.2257854	-0.1887358	0.0366341
C	-0.0105362	-2.3876313	0.2877717
C	-1.1525482	1.2773643	0.2057977
C	-2.5006921	-0.7285108	0.4267039
C	1.2060326	1.2411371	-0.0219785
C	2.5105010	-0.8051285	-0.0513538
C	-0.1207600	-3.2594085	-0.8305498
C	0.0945398	-2.9464598	1.5785344
O	0.0336501	1.9333146	0.0565355
C	-2.3007722	2.0494951	0.2938363
C	-3.6787694	0.0020595	0.5177925
C	2.3723992	1.9776360	-0.1616591
C	3.7057952	-0.1109276	-0.1902981
C	-0.1227779	-4.6570135	-0.6317902
C	-0.2350593	-2.6774636	-2.2040687
C	0.0912771	-4.3389716	1.7632437
C	-3.5869584	1.4542789	0.4495127
C	-4.9817171	-0.7509969	0.6768730
C	3.6456174	1.3430406	-0.2555167
C	4.9940078	-0.9021707	-0.2553396
C	-0.0175017	-5.1968756	0.6569244
O	-0.3268819	-3.6210508	-3.1696285
O	-0.2462660	-1.4795423	-2.4485412
N	-4.6424969	2.3156797	0.5231563
N	4.7209189	2.1713078	-0.3948852
C	-6.0841017	2.1017435	0.6906844
C	6.1529468	1.9101441	-0.5771712
C	-6.8091171	3.4458065	0.7234910
C	6.9078852	3.2301813	-0.7220491
H	-2.5649712	-1.8255966	0.4756357
H	2.5504791	-1.9033980	-0.0028859
H	0.1802375	-2.2775976	2.4483214
H	-2.2001624	3.1434391	0.2391863
H	2.2958470	3.0740242	-0.2053939
H	-0.2089603	-5.3145483	-1.5077650
H	0.1743959	-4.7526188	2.7796706
H	-5.5057767	-0.4984970	1.6195567
H	-4.7874384	-1.8396721	0.6943291
H	-5.6856153	-0.5592379	-0.1567063
H	4.7763330	-1.9833162	-0.1716190
H	5.6889355	-0.6450648	0.5683231
H	5.5380292	-0.7522734	-1.2083689
H	-0.0205111	-6.2878092	0.7981864
H	-0.3977746	-3.1377810	-4.0220083
H	-4.3790218	3.3011686	0.4500371
H	4.4786256	3.1646721	-0.4165095
H	-6.2820247	1.5481503	1.6315193
H	-6.4800022	1.4846779	-0.1422301
H	6.3158662	1.2855633	-1.4799678
H	6.5539230	1.3449953	0.2890278
H	-6.4619409	4.0736330	1.5696574
H	-7.8971573	3.2876586	0.8496235
H	-6.6606366	4.0099694	-0.2201436
H	6.5563086	3.8042641	-1.6038911
H	7.9887657	3.0365775	-0.8595447
H	6.7937841	3.8639048	0.1813471

Table 5: B3LYP/def2-SVP optimized S1 geometry of Rh575⁺ in Å.

C	-0.1157748	-0.9541964	0.1021754
C	-1.2837598	-0.1767663	0.2052275
C	1.1592211	-0.2109871	-0.0230411
C	-0.1388792	-2.4230874	0.2271635
C	-1.2153999	1.2602355	0.1447117
C	-2.6114633	-0.7104690	0.2935881
C	1.1224876	1.1841798	-0.0829389
C	2.4451802	-0.8030777	-0.0194211
C	0.3222294	-3.3159739	-0.7860709
C	-0.6148064	-2.9859541	1.4315892
O	-0.0255834	1.8977597	-0.0207228
C	-2.3386753	2.0540683	0.2479945
C	-3.7607517	0.0511214	0.3837705
C	2.2986777	1.9404421	-0.1909347
C	3.6515589	-0.1097341	-0.1138213
C	0.3266546	-4.7026757	-0.5498755
C	0.7018245	-2.7892519	-2.1225154
C	-0.6020558	-4.3627560	1.6508145
C	-3.6325563	1.4982231	0.4007891
C	-5.0943855	-0.6571849	0.3797874
C	3.5774921	1.3142416	-0.2339727
C	4.9467037	-0.8879588	-0.0309584
C	-0.1217814	-5.2281305	0.6597032
O	1.0263879	-3.7514977	-3.0058127
O	0.7190595	-1.6115739	-2.4233753
N	-4.6735396	2.3725953	0.5069052
N	4.6364413	2.1730823	-0.3841572
C	-6.0408840	2.1828491	0.9904683
C	6.0257188	1.9124985	-0.7359656
C	-6.6843834	3.5342258	1.2820230
C	6.7238302	3.2026594	-1.1500635
H	-2.7192282	-1.7948766	0.2541235
H	2.4968966	-1.8885689	0.0842583
H	-0.9627014	-2.3180357	2.2231455
H	-2.2068385	3.1380467	0.2189936
H	2.2083315	3.0272991	-0.2509885
H	0.6749123	-5.3669346	-1.3417405
H	-0.9565150	-4.7614106	2.6048106
H	-5.6419689	-0.5412171	1.3275733
H	-4.9481352	-1.7337567	0.2168465
H	-5.7482769	-0.2871683	-0.4251222
H	4.7335381	-1.9360140	0.2216699
H	5.6165787	-0.4990792	0.7511472
H	5.5081044	-0.8958424	-0.9783550
H	-0.1058460	-6.3073860	0.8275795
H	1.2343108	-3.3088309	-3.8463812
H	-4.4047816	3.3467789	0.4118373
H	4.3891909	3.1582659	-0.3492896
H	-6.0304529	1.5706884	1.9076325
H	-6.6476593	1.6414066	0.2463408
H	6.0591394	1.1784447	-1.5579519
H	6.5586510	1.4547870	0.1166634
H	-6.1321961	4.0826804	2.0625312
H	-7.7162655	3.3931795	1.6357220
H	-6.7260904	4.1604094	0.3754541
H	6.2445580	3.6528938	-2.0342054
H	7.7737637	2.9960860	-1.4039471
H	6.7201927	3.9412483	-0.3314114

Table 6: B3LYP/def2-SVP optimized T1 geometry of Rh575⁺ in Å.

C	-0.0141629	-0.9103307	0.2241884
C	-1.2159603	-0.1537486	0.3146390
C	1.2111801	-0.1906452	0.0600884
C	-0.0334966	-2.3992888	0.3149384
C	-1.1647181	1.2752860	0.2416938
C	-2.5143756	-0.7182514	0.4583425
C	1.1889991	1.2377842	-0.0084845
C	2.4881923	-0.8003952	-0.0383459
C	0.0206782	-3.2546321	-0.8172445
C	-0.1195489	-2.9879205	1.5885992
O	0.0217463	1.9332180	0.0882465
C	-2.2998930	2.0419201	0.3216995
C	-3.6914884	0.0171901	0.5416731
C	2.3417380	1.9657672	-0.1718059
C	3.6833369	-0.1073193	-0.2040267
C	-0.0063417	-4.6497795	-0.6399951
C	0.0906075	-2.6877703	-2.2007741
C	-0.1417007	-4.3756147	1.7528068
C	-3.5935865	1.4529984	0.4773330
C	-4.9936106	-0.7350270	0.6821812
C	3.6177876	1.3306056	-0.2799805
C	4.9637239	-0.9013243	-0.2904743
C	-0.0827821	-5.2105709	0.6343741
O	0.0000184	-3.6343516	-3.1545309
O	0.2163454	-1.5147689	-2.4741443
N	-4.6363306	2.3334679	0.5458693
N	4.6801783	2.1728579	-0.4470056
C	-6.0711746	2.1312004	0.7292601
C	6.1082720	1.9185507	-0.6184930
C	-6.7900350	3.4742603	0.7820496
C	6.8605825	3.2313230	-0.8018422
H	-2.5866172	-1.8058367	0.5017333
H	2.5312117	-1.8888430	0.0196201
H	-0.1637690	-2.3380024	2.4663555
H	-2.1964751	3.1277888	0.2613772
H	2.2648994	3.0542524	-0.2230621
H	0.0320164	-5.2922954	-1.5201197
H	-0.2028417	-4.8027107	2.7571736
H	-5.5190857	-0.4940793	1.6191390
H	-4.8022050	-1.8165476	0.6854670
H	-5.6870774	-0.5290094	-0.1476647
H	4.7467166	-1.9731343	-0.1896326
H	5.6761286	-0.6356097	0.5059087
H	5.4787294	-0.7618008	-1.2536768
H	-0.0986502	-6.2965825	0.7530464
H	0.0589322	-3.1783296	-4.0115692
H	-4.3614651	3.3079894	0.4651516
H	4.4279740	3.1570864	-0.4707703
H	-6.2533279	1.5710621	1.6606368
H	-6.4741570	1.5227016	-0.0968662
H	6.2669874	1.2668804	-1.4930074
H	6.4992556	1.3792443	0.2597603
H	-6.4312469	4.0890722	1.6235703
H	-7.8698532	3.3176780	0.9191730
H	-6.6509071	4.0410087	-0.1531183
H	6.5119091	3.7728479	-1.6962529
H	7.9346489	3.0331365	-0.9294412
H	6.7440885	3.8873417	0.0762330

Table 7: B3LYP/def2-SVP optimized S0 geometry of RhB⁺ in Å.

C	0.4557542	17.0407148	-1.4661486
C	0.5128942	18.5198181	-1.6891899
C	0.2867345	18.9978125	-2.9887868
C	0.3250392	20.3677190	-3.2663428
C	0.5910965	21.2825129	-2.2445337
C	0.8181368	20.8221871	-0.9474489
C	0.7824927	19.4483743	-0.6554836
C	-0.7704047	16.4074345	-1.1652216
C	-0.8044706	14.9890098	-1.0095855
C	-1.9599506	14.2942681	-0.6975931
C	-3.1891380	14.9832542	-0.5135756
C	-3.1668520	16.4168629	-0.6708910
C	-2.0111848	17.0860131	-0.9796772
C	1.6082804	16.2435785	-1.6429906
C	2.9018351	16.7471537	-1.9709640
C	3.9885726	15.9237691	-2.1113783
C	3.8814329	14.4965921	-1.9323050
C	2.5975891	13.9810854	-1.6074544
C	1.5136721	14.8301404	-1.4683739
O	0.3254666	14.2562036	-1.1599763
N	-4.3376616	14.3261422	-0.2078602
C	-5.5989555	15.0281826	0.0678380
C	-6.4461627	15.2924798	-1.1784295
C	-4.3944166	12.8611244	-0.1253093
C	-4.0462808	12.3048239	1.2571935
N	4.9633726	13.6868006	-2.0664973
C	4.8889562	12.2437945	-1.8045059
C	6.2803156	14.1914948	-2.4797165
C	7.1555564	14.6627514	-1.3168322
C	4.4788248	11.4136367	-3.0228911
C	1.0273694	18.9600711	0.7361342
O	1.2679422	19.9531787	1.6062209
O	1.0143710	17.7940419	1.0636938
H	1.0271092	21.5254376	-0.1404631
H	0.6219484	22.3536405	-2.4569980
H	0.1457701	20.7174579	-4.2861336
H	0.0780354	18.2867406	-3.7919543
H	3.0261137	17.8228273	-2.1070165
H	4.9514187	16.3721761	-2.3472702
H	2.4175468	12.9174689	-1.4713502
H	-2.0371026	18.1710234	-1.0943376
H	-4.0839655	16.9911831	-0.5577262
H	-1.8765937	13.2163605	-0.5817005
H	-5.3858044	15.9645202	0.6035528
H	-6.1632809	14.4055697	0.7791308
H	-5.9223154	15.9433502	-1.8958205
H	-7.3898826	15.7851498	-0.8960432
H	-6.6989260	14.3540987	-1.6969203
H	-4.1373786	11.2072003	1.2559533
H	-4.7271686	12.6974113	2.0289171
H	-3.0173890	12.5623293	1.5524979
H	-3.7402779	12.4299384	-0.8976485
H	-5.4167741	12.5615347	-0.4028981
H	4.4722636	10.3429072	-2.7649003
H	5.1837674	11.5537262	-3.8575750
H	3.4736188	11.6850155	-3.3809545
H	4.2070853	12.0644110	-0.9600139
H	5.8834404	11.9275601	-1.4537835
H	8.1376344	14.9910080	-1.6921182
H	7.3270173	13.8522517	-0.5908519
H	6.6960267	15.5060360	-0.7780507
H	6.1478950	14.9927597	-3.2211334
H	6.7822799	13.3732537	-3.0188349
H	1.4145532	19.5466460	2.4779492

Table 8: B3LYP/def2-SVP optimized S1 geometry of RhB⁺ in Å.

C	0.5743696	17.1142725	-1.4281637
C	0.6405412	18.5703015	-1.6551087
C	0.9606353	19.0323754	-2.9501156
C	0.9751029	20.3921420	-3.2586447
C	0.6795187	21.3400978	-2.2712486
C	0.3879603	20.9137078	-0.9775255
C	0.3684764	19.5457939	-0.6504753
C	-0.7016458	16.4473004	-1.0838879
C	-0.7209380	15.0564589	-0.9440407
C	-1.8933924	14.3415795	-0.6320377
C	-3.1260495	15.0226579	-0.4551268
C	-3.1223326	16.4359139	-0.6295404
C	-1.9470739	17.1039264	-0.9323110
C	1.6845111	16.2765504	-1.6332127
C	3.0095055	16.7361097	-1.9456905
C	4.0657273	15.8787850	-2.1226532
C	3.9177311	14.4512561	-1.9927930
C	2.6263143	13.9751482	-1.6463801
C	1.5699584	14.8502444	-1.4696885
O	0.3801397	14.2880804	-1.1167991
N	-4.2690445	14.3233315	-0.1243669
C	-5.5246394	15.0118567	0.1690763
C	-6.3903780	15.2705920	-1.0730356
C	-4.2987398	12.8640532	-0.0325776
C	-3.9355082	12.3244825	1.3581817
N	4.9753606	13.6078837	-2.1739145
C	4.8597547	12.1653371	-1.9434716
C	6.2928862	14.0821922	-2.6118598
C	7.2213776	14.4852004	-1.4629272
C	4.3824504	11.3776802	-3.1675534
C	0.1649565	19.1221429	0.7598444
O	0.0042042	20.1527011	1.6104866
O	0.1494312	17.9683118	1.1408318
H	0.1852455	21.6423238	-0.1916799
H	0.6853106	22.4064118	-2.5082522
H	1.2057481	20.7125993	-4.2778566
H	1.1624331	18.3000690	-3.7355018
H	3.1816959	17.8097700	-2.0254148
H	5.0434525	16.3068055	-2.3369481
H	2.4168064	12.9158837	-1.5147245
H	-1.9850777	18.1857869	-1.0704267
H	-4.0406903	17.0119676	-0.5406590
H	-1.7985608	13.2627523	-0.5303114
H	-5.3040864	15.9547480	0.6909241
H	-6.0810508	14.3845504	0.8828349
H	-5.8733158	15.9150615	-1.7997956
H	-7.3248634	15.7693220	-0.7719004
H	-6.6556759	14.3284104	-1.5773577
H	-4.0156190	11.2261186	1.3606160
H	-4.6166629	12.7154617	2.1298039
H	-2.9071270	12.5978601	1.6401205
H	-3.6384898	12.4350848	-0.8002577
H	-5.3191065	12.5450340	-0.2974010
H	4.3452311	10.3021082	-2.9325472
H	5.0665156	11.5123644	-4.0202603
H	3.3774971	11.6938567	-3.4872569
H	4.1971499	11.9876633	-1.0828542
H	5.8529190	11.8047930	-1.6333364
H	8.2007419	14.7951309	-1.8605503
H	7.3899393	13.6449793	-0.7708676
H	6.8068831	15.3232869	-0.8811957
H	6.1643209	14.9135483	-3.3203586
H	6.7519806	13.2674681	-3.1937619
H	-0.0978222	19.7743323	2.5005275

Table 9: B3LYP/def2-SVP optimized T1 geometry of RhB⁺ in Å.

C	0.4760362	17.0657153	-1.5116307
C	0.5465660	18.5418526	-1.7104780
C	0.5666719	19.0346444	-3.0272169
C	0.6288698	20.4046659	-3.2950479
C	0.6781379	21.3193707	-2.2402590
C	0.6705079	20.8545843	-0.9257787
C	0.6046026	19.4779262	-0.6438621
C	-0.7546313	16.4169069	-1.1747956
C	-0.7875158	14.9970986	-1.0181098
C	-1.9378568	14.3083674	-0.6922158
C	-3.1693103	15.0018435	-0.4930476
C	-3.1549515	16.4210271	-0.6554343
C	-1.9917619	17.0900818	-0.9844133
C	1.6298384	16.2486651	-1.6765681
C	2.9306975	16.7379718	-1.9929910
C	4.0212444	15.9031760	-2.1385379
C	3.9020038	14.4895523	-1.9707432
C	2.6083991	13.9817024	-1.6421045
C	1.5319739	14.8311527	-1.5026788
O	0.3378938	14.2466386	-1.1869008
N	-4.3189854	14.3277069	-0.1639609
C	-5.5775670	15.0241130	0.1301056
C	-6.4448304	15.2685180	-1.1087311
C	-4.3684228	12.8636760	-0.0777022
C	-4.0084907	12.3211880	1.3091673
N	4.9804479	13.6533343	-2.1105476
C	4.8894605	12.2128310	-1.8495297
C	6.2991148	14.1430354	-2.5290728
C	7.1852026	14.5932252	-1.3639171
C	4.4733077	11.3922169	-3.0741171
C	0.6190851	19.0159018	0.7793780
O	0.8201095	20.0232549	1.6504952
O	0.4695041	17.8722028	1.1488423
H	0.7186691	21.5592552	-0.0951194
H	0.7254798	22.3924945	-2.4399174
H	0.6357074	20.7557735	-4.3302167
H	0.5246015	18.3226043	-3.8554449
H	3.0659299	17.8130451	-2.1175634
H	4.9863114	16.3517458	-2.3674397
H	2.4222191	12.9191453	-1.5017609
H	-2.0188111	18.1735997	-1.1059968
H	-4.0682289	17.0006493	-0.5339956
H	-1.8544490	13.2296597	-0.5794940
H	-5.3557167	15.9676808	0.6472108
H	-6.1253478	14.4020440	0.8545066
H	-5.9348920	15.9165113	-1.8377818
H	-7.3851241	15.7579997	-0.8112174
H	-6.7014868	14.3236968	-1.6128412
H	-4.1005295	11.2239874	1.3124496
H	-4.6834577	12.7182452	2.0833754
H	-2.9768281	12.5819235	1.5900773
H	-3.7140936	12.4345469	-0.8491729
H	-5.3926503	12.5610374	-0.3444416
H	4.4592618	10.3213034	-2.8179366
H	5.1795727	11.5298017	-3.9078501
H	3.4701241	11.6745312	-3.4285417
H	4.2012775	12.0401620	-1.0098803
H	5.8805520	11.8854500	-1.4993006
H	8.1677267	14.9127005	-1.7449196
H	7.3522005	13.7742711	-0.6466791
H	6.7370265	15.4372183	-0.8175975
H	6.1686655	14.9545215	-3.2587291
H	6.7880280	13.3218241	-3.0757776
H	0.8098033	19.6324433	2.5410212

Table 10: B3LYP/def2-SVP optimized S0 geometry of Rh101⁺ in Å.

C	0.4361286	-1.2790533	-0.2307333
C	-0.9476953	-0.9609545	-0.2350196
C	1.3875618	-0.2297831	-0.1450274
C	0.8891200	-2.6962261	-0.4027569
C	-1.3506368	0.4077170	-0.1094340
C	-1.9938437	-1.9246419	-0.3514993
C	0.9291401	1.1202535	-0.0126475
C	2.8006563	-0.4268572	-0.1407206
C	0.9751688	-3.6082659	0.6856221
C	1.2317393	-3.1418979	-1.6963367
C	-2.6863929	0.8188296	-0.0960418
O	-0.4108727	1.3940911	0.0009395
C	-3.3328969	-1.5804647	-0.3236687
C	1.7871315	2.2151644	0.1202909
C	3.6990232	0.6182664	-0.0329980
C	1.4356077	-4.9220390	0.4495315
C	0.6256251	-3.1289900	2.0738454
C	1.6733792	-4.4569565	-1.9166302
C	-3.7074450	-0.1834482	-0.1932587
C	-3.0387708	2.2857125	0.0293634
C	-4.4115761	-2.6402194	-0.3962474
C	3.2011076	1.9754583	0.1068547
C	1.2314004	3.6141029	0.2813248
C	5.1917460	0.3710187	-0.0778402
C	1.7842019	-5.3495696	-0.8394955
O	0.3123827	-4.0807718	2.9876094
O	0.6152144	-1.9540990	2.3859345
N	-5.0310539	0.1737681	-0.1710536
C	-4.4504049	2.5588104	-0.4950599
C	-5.7009163	-2.0720335	-0.9920858
N	4.0802211	3.0197739	0.2326141
C	2.2576255	4.5397100	0.9388686
C	5.9490682	1.4508019	0.6972609
C	-5.4359576	1.5581599	0.1017525
C	-6.1104096	-0.8207855	-0.2218457
C	3.6076320	4.4094748	0.2392510
C	5.5358324	2.8281383	0.1887123
H	-1.7194241	-2.9845940	-0.4597493
H	3.1855091	-1.4534334	-0.2292867
H	1.1507011	-2.4420757	-2.5418819
H	1.5641424	-5.6226457	1.2910606
H	1.9382085	-4.7808150	-2.9343454
H	-2.9625700	2.5964796	1.0962582
H	-2.2921913	2.8978015	-0.5142066
H	-4.0474567	-3.5106950	-0.9781319
H	-4.6193476	-3.0202640	0.6302719
H	0.9393114	4.0173937	-0.7150658
H	0.2971862	3.5786375	0.8758437
H	5.4182570	-0.6407379	0.3140280
H	5.5323226	0.3747367	-1.1387727
H	2.1492631	-6.3747557	-0.9995114
H	0.2576504	-4.9575105	2.5572730
H	-4.7729920	3.5881625	-0.2424054
H	-4.4705879	2.4742075	-1.6023226
H	-5.5499278	-1.8169202	-2.0626574
H	-6.5230252	-2.8133832	-0.9467049
H	1.9218819	5.5947260	0.8971984
H	2.3760640	4.2778751	2.0115927
H	5.7253362	1.3720881	1.7824018
H	7.0445670	1.3329537	0.5807280
H	-6.4484379	1.7001026	-0.3265586
H	-5.5307634	1.7117581	1.2030678
H	-6.4236421	-1.0880589	0.8156481
H	-6.9859125	-0.3354311	-0.6997166
H	3.5440709	4.7896731	-0.8081185
H	4.3768996	5.0207757	0.7520732
H	5.9032071	2.9841300	-0.8538148
H	5.9938590	3.6276241	0.8064302

Table 11: B3LYP/def2-SVP optimized S1 geometry of Rh101⁺ in Å.

C	0.3477491	-1.3602488	-0.1698680
C	-1.0058742	-0.9980217	-0.2260760
C	1.3369069	-0.2708440	-0.0408591
C	0.7863754	-2.7629126	-0.3581472
C	-1.3958414	0.3840290	-0.1216747
C	-2.0903628	-1.9269739	-0.3339408
C	0.8756919	1.0358144	0.0699428
C	2.7417168	-0.4484742	-0.0402790
C	1.4143869	-3.5446154	0.6543280
C	0.5930414	-3.3548042	-1.6232896
C	-2.7112259	0.8281751	-0.1660165
O	-0.4385434	1.3461980	0.0400715
C	-3.4101646	-1.5395161	-0.3611650
C	1.7488147	2.1561817	0.2241881
C	3.6535651	0.5910818	0.0739710
C	1.8845377	-4.8335342	0.3408398
C	1.5306257	-3.0043123	2.0483025
C	1.0502970	-4.6410684	-1.9113271
C	-3.7543404	-0.1356362	-0.2896486
C	-3.0255266	2.3056998	-0.0692073
C	-4.5126051	-2.5715885	-0.4239714
C	3.1645001	1.9216031	0.2157782
C	1.1824049	3.5362598	0.3782773
C	5.1445976	0.3322960	0.0501527
C	1.7164687	-5.3818063	-0.9291948
O	1.6877457	-3.9006260	3.0422199
O	1.4791708	-1.8255588	2.3098198
N	-5.0672483	0.2570118	-0.3396939
C	-4.4063498	2.6135806	-0.6455583
C	-5.7661274	-1.9988037	-1.0806122
N	4.0239601	2.9909062	0.3495083
C	2.1872035	4.4924143	1.0173935
C	5.8963698	1.4313605	0.7987786
C	-5.4398470	1.6464096	-0.0834254
C	-6.1651786	-0.7086481	-0.3781810
C	3.5374671	4.3665609	0.3257058
C	5.4705694	2.8007684	0.2814685
H	-1.8567277	-2.9918070	-0.3781581
H	3.1303430	-1.4639678	-0.1395486
H	0.1009628	-2.7709815	-2.4050626
H	2.4176833	-5.4188355	1.0962534
H	0.9034719	-5.0582998	-2.9107177
H	-2.9807963	2.6248327	0.9890696
H	-2.2517697	2.8878833	-0.5917677
H	-4.1568358	-3.4687503	-0.9537273
H	-4.7586903	-2.8982735	0.6044138
H	0.8915991	3.9104262	-0.6254753
H	0.2440211	3.4936669	0.9512223
H	5.3590372	-0.6534413	0.4912606
H	5.5030296	0.2874749	-0.9952668
H	2.1027417	-6.3791264	-1.1513079
H	1.5580272	-4.8049782	2.7231327
H	-4.7054207	3.6467559	-0.4112499
H	-4.3872051	2.5220110	-1.7448807
H	-5.5776756	-1.7946601	-2.1485674
H	-6.6010451	-2.7142287	-1.0285143
H	1.8331325	5.5319100	0.9473908
H	2.3023887	4.2579320	2.0890612
H	5.6850581	1.3684913	1.8797203
H	6.9847474	1.3256964	0.6737057
H	-6.4242726	1.8204951	-0.5440112
H	-5.5655213	1.8097113	1.0069527
H	-6.5108583	-0.9275006	0.6532518
H	-7.0111032	-0.2311972	-0.8975057
H	3.4651378	4.7199332	-0.7251316
H	4.2915963	4.9981781	0.8184487
H	5.8089146	2.9350775	-0.7676276
H	5.9410986	3.6072143	0.8660265

Table 12: B3LYP/def2-SVP optimized T1 geometry of Rh101⁺ in Å.

C	0.4155851	-1.2951093	-0.2768833
C	-0.9664088	-0.9618209	-0.2778563
C	1.3689124	-0.2318628	-0.1467948
C	0.8619152	-2.7118104	-0.4257694
C	-1.3690333	0.4052338	-0.1507152
C	-2.0191454	-1.9129931	-0.3883636
C	0.9095044	1.1102526	-0.0043855
C	2.7728333	-0.4257592	-0.1467171
C	1.2170015	-3.5301529	0.6776056
C	0.9132875	-3.2766128	-1.7125070
C	-2.6902660	0.8175525	-0.1548682
O	-0.4280218	1.3925901	-0.0178386
C	-3.3568866	-1.5616754	-0.3761627
C	1.7607596	2.1909792	0.1652978
C	3.6742084	0.6133953	-0.0039929
C	1.6377761	-4.8540289	0.4563826
C	1.1769641	-2.9860890	2.0825131
C	1.3301234	-4.5944793	-1.9203523
C	-3.7211625	-0.1781258	-0.2592625
C	-3.0363218	2.2832668	-0.0293609
C	-4.4327916	-2.6201900	-0.4517536
C	3.1774392	1.9515212	0.1591846
C	1.2060799	3.5836287	0.3435797
C	5.1617718	0.3578029	-0.0357068
C	1.7028675	-5.3861289	-0.8319577
O	0.8517337	-3.8719721	3.0483335
O	1.4234642	-1.8432944	2.3700551
N	-5.0438271	0.1958178	-0.2484846
C	-4.4410722	2.5691830	-0.5552353
C	-5.7246523	-2.0520501	-1.0334948
N	4.0510782	3.0015801	0.3086859
C	2.2221129	4.5031886	1.0164312
C	5.9192659	1.4303769	0.7420904
C	-5.4350314	1.5770922	0.0323225
C	-6.1212437	-0.7948158	-0.2719608
C	3.5743649	4.3858932	0.3275284
C	5.5027404	2.8101375	0.2528080
H	-1.7556658	-2.9679649	-0.4815876
H	3.1542653	-1.4422020	-0.2519584
H	0.6261507	-2.6592263	-2.5676394
H	1.9516065	-5.4726050	1.3024800
H	1.3699286	-4.9990969	-2.9348896
H	-2.9643134	2.5857631	1.0328203
H	-2.2887401	2.8880732	-0.5632119
H	-4.0738131	-3.4770629	-1.0425017
H	-4.6301606	-3.0091635	0.5654379
H	0.9236885	3.9936919	-0.6451648
H	0.2734905	3.5378341	0.9245349
H	5.3753118	-0.6462781	0.3610351
H	5.5070034	0.3537334	-1.0875760
H	2.0468520	-6.4120286	-0.9833599
H	0.5623979	-4.7114765	2.6626223
H	-4.7541384	3.5928224	-0.2989153
H	-4.4591575	2.4900862	-1.6556016
H	-5.5870472	-1.8068972	-2.1004753
H	-6.5437538	-2.7846618	-0.9714291
H	1.8878790	5.5511798	0.9805144
H	2.3332724	4.2339962	2.0804685
H	5.7042585	1.3420757	1.8205400
H	7.0070631	1.3192704	0.6169966
H	-6.4398555	1.7318831	-0.3885064
H	-5.5219849	1.7201404	1.1286280
H	-6.4069266	-1.0497098	0.7688642
H	-7.0005127	-0.3186530	-0.7326675
H	3.5137608	4.7600052	-0.7143355
H	4.3347312	4.9930337	0.8402367
H	5.8442182	2.9708037	-0.7898190
H	5.9642662	3.6021128	0.8620652