

Supporting Information for:

**Anion-Regulated Electronic Communication in a Cyclometalated
Diruthenium Complex with a Urea Bridge**

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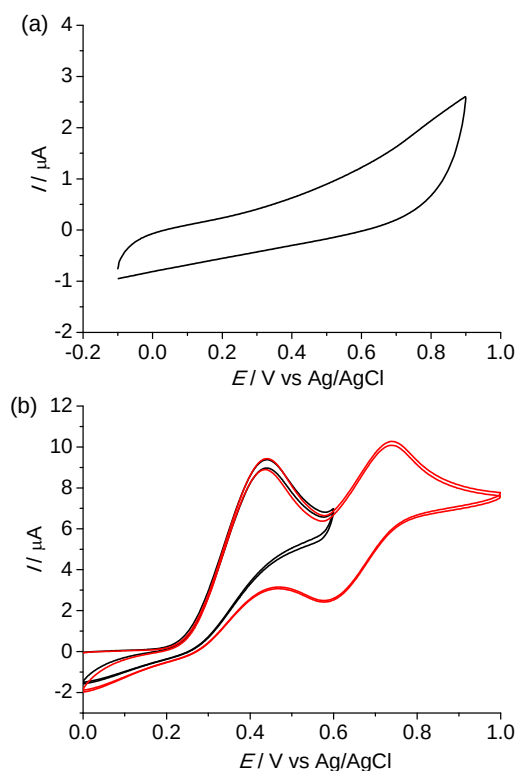


Figure S1. CV of (a) $\text{Bu}_4\text{NH}_2\text{PO}_4$ and (b) Bu_4NI . The CV of Bu_4NI shows a two-step EC_1EC_2 response. The black line shows the first step process, which is ascribed to the oxidation of iodide followed by the formation of triiodide. The second step is due to the further oxidation of triiodide followed by the formation of iodine.¹

¹ (a) I. S. El-Hallag, *J. Chil. Chem. Soc.*, 2010, **55**, 67; (b) Y. A. Yaraliyev. *Electrochimica Acta*, 1984, **29**, 1213.

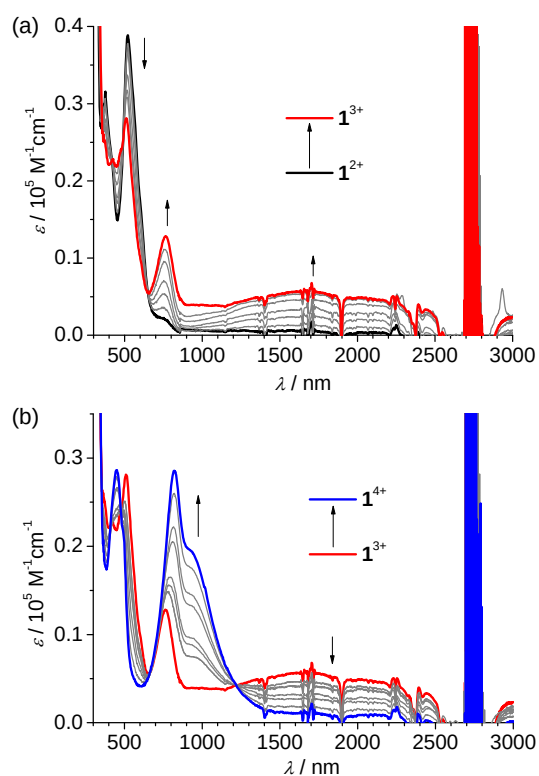


Figure S2. Absorption spectral changes of $\mathbf{1}(\text{PF}_6)_2$ upon stepwise oxidation with $(p\text{-BrC}_6\text{H}_4)_4\text{NSbCl}_6$ in CH_2Cl_2 . Up to 1.0 equiv of $(p\text{-BrC}_6\text{H}_4)_4\text{NSbCl}_6$ was used in step (a) and up to 2.0 equiv of $(p\text{-BrC}_6\text{H}_4)_4\text{NSbCl}_6$ was used in step (b).

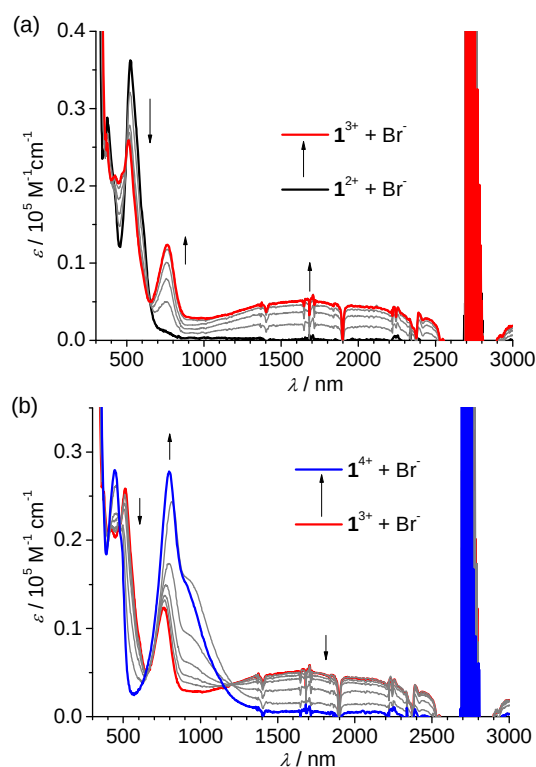


Figure S3. Absorption spectral changes of $1(\text{PF}_6)_2$ in the presence of 5 equiv of Bu_4NBr upon stepwise oxidation with $(p\text{-BrC}_6\text{H}_4)_4\text{NSbCl}_6$ in CH_2Cl_2 . Up to 1.0 equiv of $(p\text{-BrC}_6\text{H}_4)_4\text{NSbCl}_6$ was used in step (a) and up to 10.0 equiv of $(p\text{-BrC}_6\text{H}_4)_4\text{NSbCl}_6$ was used in step (b). Due to the relative high oxidation potential of the second-step oxidation, an excess amount of $(p\text{-BrC}_6\text{H}_4)_4\text{NSbCl}_6$ was used for complete transformation.

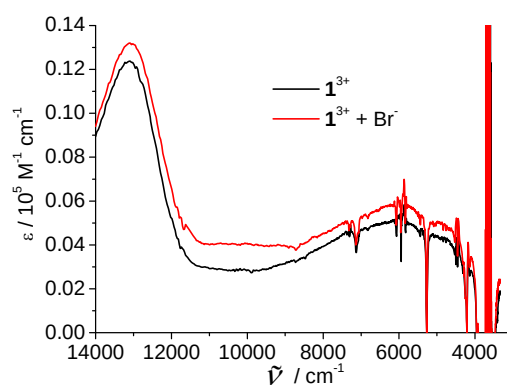


Figure S4 A comparison of the absorption spectra of 1^{3+} (recorded during the chemical oxidation experiments) as a function of wavenumbers in the absence or presence of 5 eq Br^- in CH_2Cl_2 .

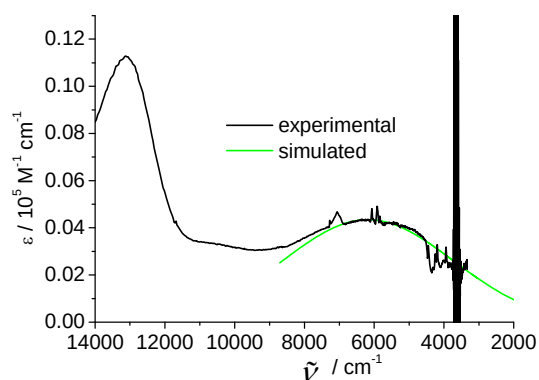


Figure S5 Near-infrared absorption spectra (black curve) and Gaussian-fitted IVCT band (green curve) of $[1\cdots\text{Br}]^{2+}$ (recorded during spectroelectrochemical experiments).

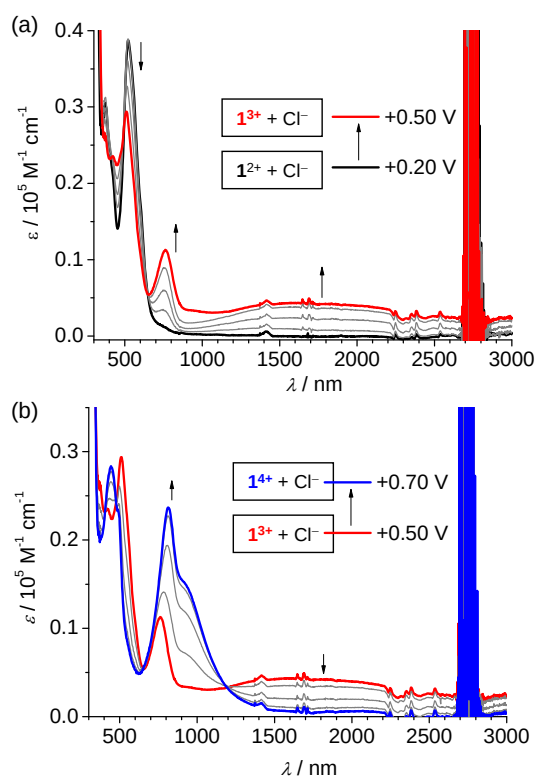


Figure S6 Absorption spectral changes of $1(\text{PF}_6)_2$ in the presence of 5 equiv of Bu_4NCl recorded during the spectroelectrochemical measurements at a transparent ITO glass electrode in 0.1 M $\text{Bu}_4\text{NPF}_6/\text{CH}_2\text{Cl}_2$. The potential was referenced vs Ag/AgCl .

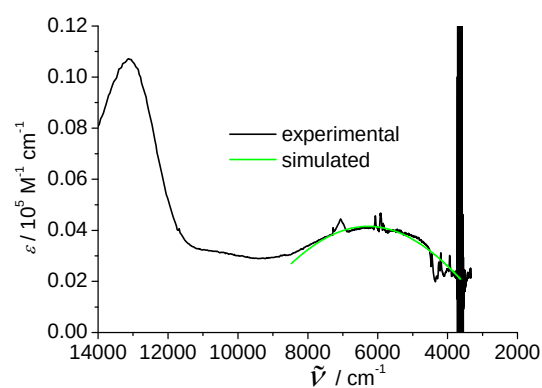


Figure S7. Near-infrared absorption spectra (black curve) and Gaussian-fitted IVCT band (green curve) of $[1\cdots\text{Cl}]^{2+}$ (recorded during spectroelectrochemical experiments).

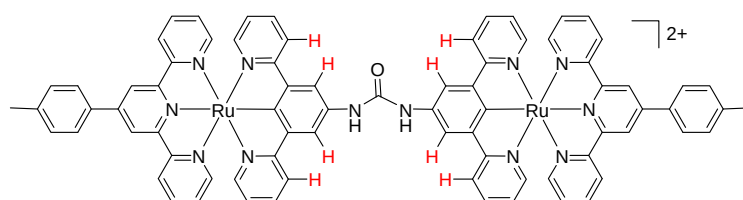


Figure S8. Complex 1^{2+} with protons close to the urea group highlighted in red.

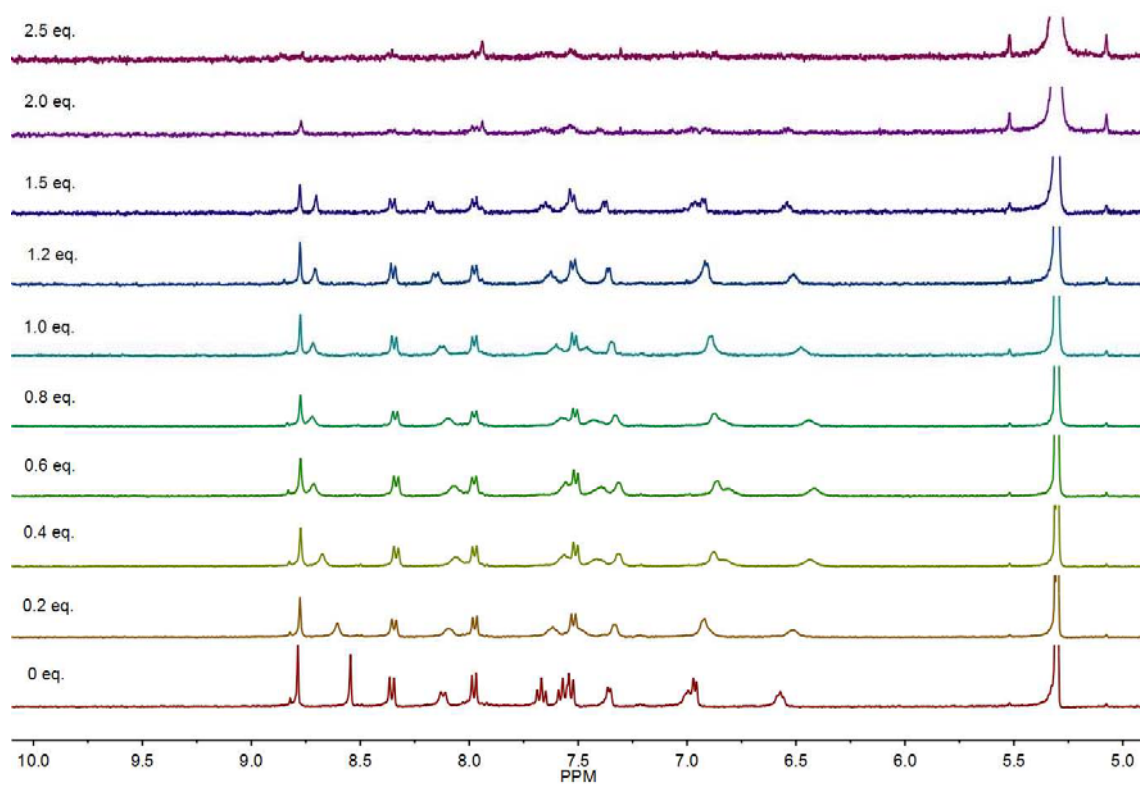


Figure S9 ^1H NMR spectral changes of $\mathbf{1}(\text{PF}_6)_2$ in CD_2Cl_2 in response to different equiv of $\text{Bu}_4\text{NH}_2\text{PO}_4$.

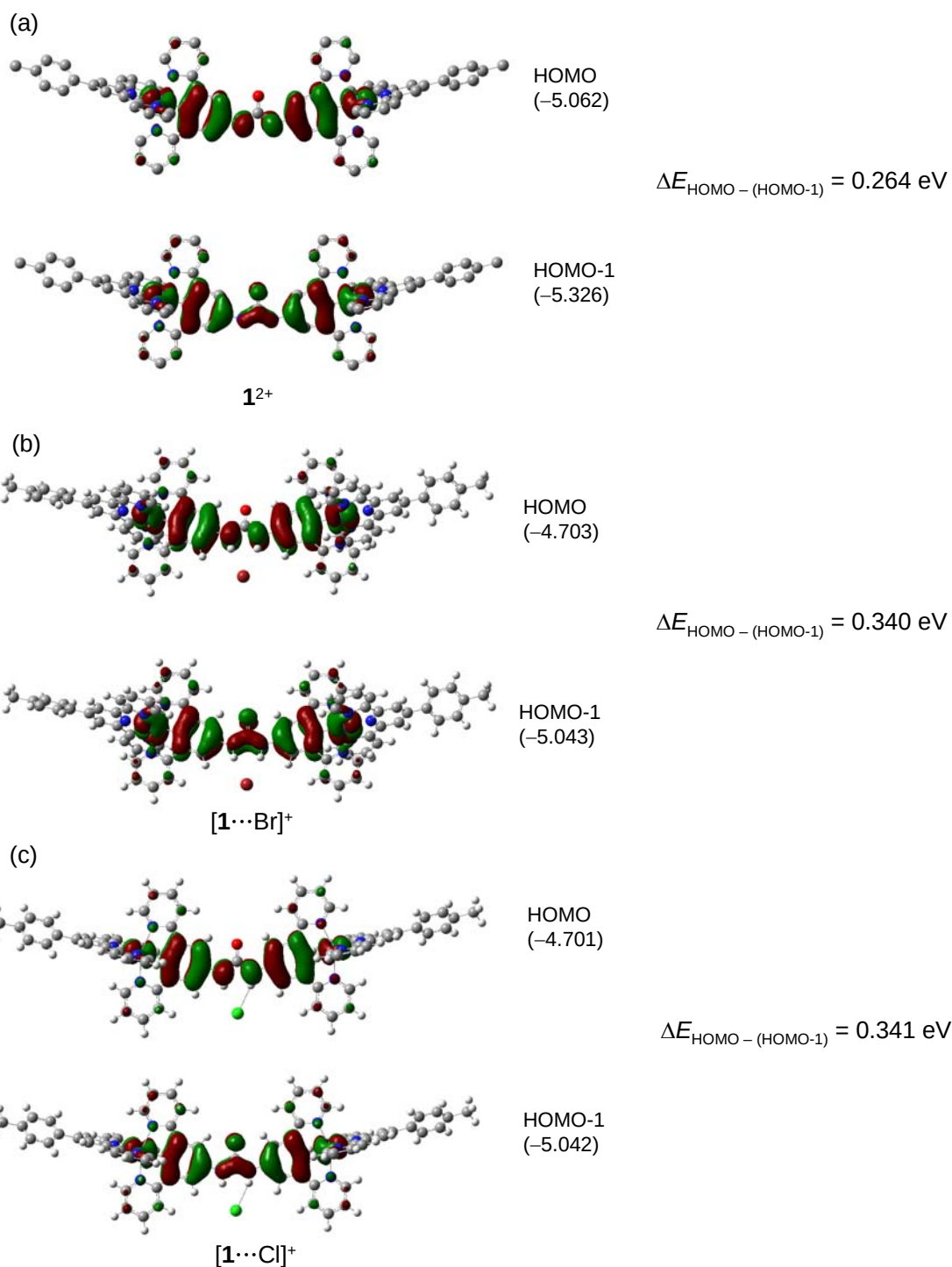


Figure S10 DFT-calculated HOMO and HOMO-1 plots of $\mathbf{1}^{2+}$, $[\mathbf{1} \cdots \text{Br}]^+$, and $[\mathbf{1} \cdots \text{Cl}]^+$.

Cartesian coordinates of DFT-optimized structure of $\mathbf{1}^{2+}$:

Charge = 2; multiplicity=1

O	13.96125193	16.74300427	3.30310892
N	12.49897913	15.79537413	4.81592715
H	11.92609338	15.98885504	5.62628781
C	12.30330505	11.72392640	3.70664614
C	11.60942286	12.20774744	4.83346583
C	11.69800624	13.56150889	5.17911690
H	11.17403752	13.95475945	6.04863275
C	12.47445833	14.44202094	4.40005953
C	13.16883392	13.96809408	3.27148525
H	13.75611938	14.66912858	2.69502685
C	13.07915843	12.60909981	2.93470904
C	13.21077767	16.85051044	4.27491915
N	12.98755293	18.03911345	4.94600599
H	12.33380783	18.02064845	5.71738017
C	14.50867796	21.92430614	4.28202802
C	13.56737567	21.67289049	5.29977307
C	13.07965163	20.37498089	5.49403181
H	12.34968209	20.16020086	6.27217902
C	13.52942250	19.31939642	4.67647111
C	14.47162179	19.56084476	3.65929949
H	14.79687868	18.73029689	3.04862957
C	14.95272218	20.86467950	3.46865867
C	10.84649601	11.16451572	5.53081424
C	10.06535991	11.35907927	6.67775068
C	9.38767224	10.29069136	7.25391617
H	9.99407756	12.35051766	7.11182096
C	10.28384084	8.88554304	5.53475147
C	9.49769660	9.02516529	6.67264480
H	8.78251598	10.44139596	8.14270354
H	10.39840761	7.92230042	5.04921967
H	8.98819078	8.16181922	7.08640336
C	13.73707567	11.94943973	1.79864305
C	14.57185140	12.58106945	0.86672565
C	15.14242963	11.85194977	-0.17017166
H	14.76812669	13.64331573	0.96319692
C	14.03710245	9.90622017	0.68131865
C	14.87142473	10.48485453	-0.26797226
H	15.78934733	12.34134221	-0.89193903
H	13.79809531	8.84864086	0.64555193
H	15.29365319	9.87518181	-1.05930989
C	15.92592983	21.29213867	2.45484518
C	16.53415325	20.45361800	1.51093693
C	17.44063404	20.97272167	0.59378801
H	16.28994568	19.39692973	1.50333448
C	17.10400809	23.12655425	1.58390547
C	17.73389682	22.33833776	0.62786346
H	17.91183495	20.32305733	-0.13754762
H	17.29973859	24.19151976	1.64874502
H	18.43393958	22.78859187	-0.06738532
C	13.20492968	22.87735188	6.05769068
C	12.29408186	22.92479738	7.12146607
C	12.03076850	24.12819868	7.76588955

H	11.79632250	22.01458675	7.43817526
C	13.57995511	25.18434471	6.27679059
C	12.68632942	25.28473604	7.33686862
H	11.32499994	24.16463523	8.59020276
H	14.11150477	26.05549836	5.90887825
H	12.51355987	26.24594592	7.80842344
Ru	12.18091773	9.81469970	3.21123590
Ru	15.19641259	23.75510591	3.99746700
C	17.03311168	26.06235295	4.35612187
C	15.27150935	26.49108172	2.84122785
C	17.54656532	27.34473660	4.16286145
C	15.74284176	27.78507277	2.61885911
C	16.89994438	28.23279773	3.28319178
H	18.45407277	27.65782135	4.66496210
H	15.21446573	28.45917870	1.95552965
C	12.94043726	6.94229967	3.19683732
C	11.05957262	7.42275414	1.85088196
C	12.86528621	5.58938812	2.86524020
C	10.94779504	6.08199399	1.48314669
C	11.85772273	5.13695535	1.99284286
H	13.56215989	4.87760063	3.29119582
H	10.18028974	5.76340034	0.78839005
C	17.58866391	25.01023899	5.23780265
C	18.73220526	25.19473108	6.01978624
C	19.19766851	24.15994773	6.82633777
H	19.25500486	26.14372158	5.99818676
C	17.37172452	22.82164989	6.03727285
C	18.50446658	22.94993193	6.83466856
H	20.08488857	24.29843045	7.43554890
H	16.79965005	21.90159026	6.00978436
H	18.82820838	22.11448647	7.44570736
C	14.07553686	25.86676645	2.22976287
C	13.24656101	26.53143112	1.32187918
C	12.13837987	25.88072900	0.78654195
H	13.46721522	27.55292281	1.03485822
C	12.73671138	23.95311382	2.08023825
C	11.87845272	24.56635569	1.17309262
H	11.49193514	26.39251246	0.08111841
H	12.57701563	22.93363909	2.41146007
H	11.02795539	24.01775690	0.78345541
C	13.93079074	7.57976732	4.09462784
C	14.95178781	6.86958944	4.73193816
C	15.84837124	7.53546508	5.56302166
H	15.04472435	5.80082386	4.57814562
C	14.67183331	9.56805998	5.08124857
C	15.70557461	8.91115818	5.74114044
H	16.64261411	6.98835396	6.06031143
H	14.52030166	10.63593268	5.18673264
H	16.37919221	9.47392882	6.37801770
C	10.19303911	8.53800408	1.40575123
C	9.11612758	8.36701389	0.53146161
C	8.34746889	9.46393615	0.15201385
H	8.88029841	7.38075498	0.14897487
C	9.75483023	10.83364351	1.52685289
C	8.67385108	10.72157864	0.65839494

H	7.51068038	9.33634464	-0.52695907
H	10.04836374	11.78848798	1.94692470
H	8.10587889	11.60595183	0.39102208
N	13.84385374	24.02611446	5.64422660
N	16.22548549	22.63662423	2.47803620
N	10.94426326	9.91131921	4.96651105
N	13.47840907	10.60040705	1.68997832
N	10.50474631	9.78059767	1.90211708
N	13.79819723	8.93519574	4.27600063
N	13.81112831	24.57161244	2.60462915
N	16.91109340	23.81504100	5.25415080
C	11.75740728	3.70596867	1.62108092
C	10.50741426	3.09752184	1.41134241
C	12.90926841	2.91638681	1.46213541
C	10.41698194	1.75301190	1.05929078
H	9.59542241	3.67202686	1.54784332
C	12.81131542	1.57292313	1.10666013
H	13.89244841	3.36215317	1.58413834
C	11.56537251	0.96318385	0.90173414
H	9.43646661	1.30746117	0.90963070
H	13.71983058	0.99003478	0.97655116
C	17.42514095	29.60067631	3.06206516
C	17.34217040	30.21340721	1.80032440
C	18.02021177	30.32578419	4.10968364
C	17.83952171	31.49905444	1.59624843
H	16.90939771	29.67304013	0.96303167
C	18.51131995	31.61165500	3.89937846
H	18.07089240	29.89478514	5.10569777
C	18.43562618	32.22256431	2.63857975
H	17.76910102	31.94538910	0.60740039
H	18.95328911	32.15458287	4.73135293
C	11.46159985	-0.50044761	0.54547249
H	11.34682971	-1.11754171	1.44662034
H	10.59422346	-0.69654012	-0.09344366
H	12.35857047	-0.84951793	0.02393287
C	18.99890858	33.60474560	2.41006012
H	20.08171752	33.56348496	2.23198773
H	18.54229132	34.08474260	1.53878944
H	18.83995929	34.24989395	3.28075166
N	12.04380960	7.81555188	2.68861405
N	15.92138690	25.67104109	3.69577117

Cartesian coordinates of DFT-optimized structure of $[\mathbf{1} \cdots \text{Br}]^+$:

Charge = 1; multiplicity=1

O	14.06859484	16.72695321	3.18135395
N	12.64541439	15.77777963	4.74259145
H	12.07609671	16.00391887	5.56410351
C	12.37529734	11.70844548	3.66330745
C	11.67415733	12.22114690	4.77254403
C	11.78492958	13.57592220	5.10486457
H	11.25437748	13.99908979	5.95518724
C	12.59742648	14.43263900	4.33180367
C	13.30134160	13.92739660	3.22175477
H	13.91513000	14.61031740	2.65013442
C	13.18415286	12.56654274	2.89587091
C	13.34139952	16.82807460	4.17712822
N	13.12349730	18.00422220	4.86660562
H	12.48512247	17.94668984	5.66664155
C	14.56484018	21.91822976	4.23505002
C	13.64296139	21.63272816	5.26151567
C	13.18168018	20.32417204	5.44369309
H	12.46909554	20.07441096	6.22708105
C	13.63834347	19.28698326	4.60240289
C	14.56086272	19.56432907	3.57530886
H	14.89090740	18.74772015	2.94756653
C	15.01640967	20.88065669	3.39875092
C	10.87613618	11.20448363	5.46851621
C	10.08286959	11.43180013	6.60160038
C	9.36952109	10.38742803	7.17803379
H	10.03160782	12.42959257	7.02359637
C	10.25565273	8.94028843	5.48881069
C	9.45562944	9.11263776	6.61222044
H	8.75510127	10.56383927	8.05573532
H	10.35308300	7.96903699	5.01535984
H	8.91755551	8.26729626	7.02717483
C	13.84308681	11.87946561	1.77858381
C	14.70689103	12.48121661	0.85224485
C	15.27560502	11.72847468	-0.16809575
H	14.92577642	13.53963488	0.94170128
C	14.11247168	9.81799378	0.68543368
C	14.97427128	10.36667655	-0.25678733
H	15.94461228	12.19534622	-0.88478848
H	13.84912874	8.76584113	0.65663481
H	15.39398959	9.73920828	-1.03552139
C	15.96884172	21.34228785	2.38208904
C	16.58016029	20.53102393	1.41548455
C	17.46767595	21.08053630	0.49812078
H	16.35190540	19.47105365	1.39202526
C	17.10897670	23.21050796	1.53031625
C	17.74057382	22.45011957	0.55338715
H	17.94049561	20.45136757	-0.25005660
H	17.28887505	24.27718467	1.61255469
H	18.42591482	22.92364203	-0.14114708
C	13.26875063	22.81734043	6.04333764
C	12.37003922	22.82931719	7.11893871
C	12.09202034	24.01657673	7.78608560

H	11.89435761	21.90391906	7.42506961
C	13.60242133	25.12753610	6.29708549
C	12.72002182	25.19312397	7.36893813
H	11.39580787	24.02535117	8.61928454
H	14.11365587	26.01433742	5.93756670
H	12.53453291	26.14285203	7.85875232
Ru	12.21448731	9.79464960	3.18690999
Ru	15.21779283	23.76790935	3.97472161
C	17.02216067	26.09591909	4.35135724
C	15.24026159	26.52005132	2.85781764
C	17.51798409	27.38656436	4.16717692
C	15.69415237	27.82196923	2.64533194
C	16.85249904	28.27607353	3.30315587
H	18.42670943	27.70485426	4.66389436
H	15.15142956	28.49665117	1.99415602
C	12.90902049	6.90726951	3.21548585
C	11.06111581	7.41581546	1.83328769
C	12.80941927	5.55328506	2.89494968
C	10.92575592	6.07415920	1.47668663
C	11.80630898	5.11468234	2.01047193
H	13.48314981	4.83037037	3.33915960
H	10.16265502	5.76569247	0.77231498
C	17.59892275	25.04053497	5.21517460
C	18.74248310	25.23200612	5.99567094
C	19.22690619	24.19361107	6.78620788
H	19.24968340	26.18972375	5.98616374
C	17.41892581	22.83765089	5.98545671
C	18.55255297	22.97284165	6.78040016
H	20.11380339	24.33757628	7.39468483
H	16.86042029	21.90963582	5.94765234
H	18.89088202	22.13439512	7.37931038
C	14.04595008	25.88769123	2.25176807
C	13.19606750	26.55321359	1.36390699
C	12.08961153	25.89483136	0.83448857
H	13.39905529	27.58166264	1.08865920
C	12.73105585	23.95772148	2.09329583
C	11.85244529	24.57182543	1.20645953
H	11.42660080	26.40737970	0.14511040
H	12.58969271	22.93180126	2.41278113
H	11.00384263	24.01712813	0.82134966
C	13.89704156	7.53191838	4.12447738
C	14.88987804	6.80630450	4.78863050
C	15.78333419	7.46094449	5.63187413
H	14.96293286	5.73429998	4.64644524
C	14.66032497	9.51362817	5.10837804
C	15.66578222	8.84095742	5.79545758
H	16.55551921	6.90195720	6.15032971
H	14.52837462	10.58521326	5.20192065
H	16.33712585	9.39525942	6.44211297
C	10.22635981	8.54547638	1.36488174
C	9.15701472	8.38974126	0.47842823
C	8.41689091	9.49938960	0.07986353
H	8.90449272	7.40490457	0.10277877
C	9.83619345	10.85137159	1.46044294
C	8.76375363	10.75432720	0.57968063

H	7.58568432	9.38376358	-0.60810859
H	10.14465516	11.80311989	1.87689121
H	8.21774193	11.64816250	0.29842452
N	13.88020986	23.98510994	5.64197935
N	16.24807051	22.69118637	2.42506513
N	10.95104514	9.94259962	4.92022878
N	13.55493429	10.53520506	1.67862885
N	10.55897073	9.78582504	1.85375238
N	13.79052411	8.89187681	4.29016452
N	13.80420387	24.58368874	2.61178068
N	16.94012486	23.83461199	5.21763134
C	11.68027705	3.68210395	1.65215920
C	10.42052383	3.09738669	1.43513723
C	12.81703186	2.86663618	1.51537919
C	10.30581445	1.75064563	1.09804162
H	9.51951670	3.69253519	1.55461369
C	12.69501935	1.52131346	1.17495827
H	13.80772311	3.29354443	1.64398157
C	11.43873960	0.93510686	0.96345737
H	9.31788932	1.32391652	0.94246719
H	13.59259779	0.91809432	1.06208385
C	17.36094137	29.65186468	3.09065210
C	17.26021450	30.27610000	1.83583909
C	17.95840074	30.37316418	4.13950483
C	17.74269063	31.56866919	1.63964624
H	16.82493668	29.73944966	0.99747883
C	18.43492105	31.66587958	3.93720521
H	18.02276685	29.93288151	5.13063556
C	18.34147126	32.28811038	2.68322881
H	17.65841926	32.02378920	0.65584489
H	18.87911640	32.20509813	4.77046234
C	11.30886141	-0.53082971	0.62515453
H	11.21324961	-1.13787646	1.53536331
H	10.42212375	-0.72348581	0.01243739
H	12.18725479	-0.89534809	0.08268281
C	18.88938545	33.67781842	2.46242001
H	19.96958211	33.64833441	2.26680845
H	18.41501017	34.16404521	1.60412107
H	18.73853861	34.31143906	3.34295617
N	12.04012107	7.79524147	2.68398982
N	15.90866045	25.69810390	3.69683146
Br	10.95414511	17.17915094	7.39536969

Cartesian coordinates of DFT-optimized structure of [1·Cl]⁺:

Charge = 2; multiplicity=1

O	14.04163416	16.73107619	3.20819433
N	12.60759160	15.78466935	4.76100822
H	12.03490471	16.01311496	5.57943007
C	12.35586675	11.71431892	3.67626006
C	11.65421095	12.22156934	4.78754089
C	11.75902122	13.57639042	5.12232475
H	11.22753713	13.99305649	5.97510553
C	12.56547682	14.43930335	4.34978840
C	13.26959996	13.93880735	3.23738373
H	13.87900852	14.62556062	2.66583399
C	13.15896148	12.57807695	2.90921637
C	13.30881654	16.83384040	4.19983589
N	13.08957063	18.01133032	4.88720017
H	12.44804995	17.95378986	5.68439428
C	14.55087503	21.91818647	4.24717728
C	13.62512304	21.64034751	5.27205466
C	13.15723330	20.33443099	5.45732390
H	12.44086007	20.09347605	6.23960075
C	13.61076942	19.29148883	4.62157307
C	14.53762337	19.56191126	3.59612046
H	14.86585054	18.74190751	2.97204381
C	14.99961564	20.87540190	3.41594907
C	10.86283473	11.19940972	5.48316817
C	10.07058521	11.42004948	6.61830052
C	9.36431859	10.37062168	7.19427271
H	10.01450105	12.41669308	7.04237380
C	10.25506736	8.93162940	5.50059943
C	9.45646189	9.09735343	6.62600233
H	8.75074117	10.54199007	8.07356182
H	10.35712242	7.96179387	5.02520821
H	8.92409296	8.24821424	7.04056264
C	13.81955440	11.89667096	1.78937950
C	14.67894466	12.50461170	0.86298163
C	15.24986166	11.75681815	-0.15977449
H	14.89271290	13.56391152	0.95432766
C	14.09758645	9.83880823	0.69154791
C	14.95521847	10.39370852	-0.25083846
H	15.91544789	12.22851246	-0.87649628
H	13.83944088	8.78541159	0.66104124
H	15.37689145	9.76994216	-1.03149059
C	15.95630122	21.32897184	2.39956969
C	16.56633824	20.51138146	1.43750875
C	17.45793522	21.05365383	0.51978357
H	16.33388575	19.45224526	1.41785527
C	17.10573279	23.18918540	1.54267685
C	17.73621425	22.42234570	0.57007740
H	17.92975802	20.41959032	-0.22488346
H	17.28969866	24.25546655	1.62103048
H	18.42482519	22.89032556	-0.12497935
C	13.25422376	22.82941610	6.04874451
C	12.35322202	22.84944969	7.12231899
C	12.07905540	24.04032604	7.78458464

H	11.87267362	21.92739072	7.43086759
C	13.59759614	25.13908121	6.29487813
C	12.71320961	25.21252864	7.36457999
H	11.38108145	24.05519339	8.61622182
H	14.11341796	26.02235837	5.93323798
H	12.53091472	26.16485395	7.85053404
Ru	12.20394117	9.80081420	3.19611866
Ru	15.21205057	23.76403546	3.98105960
C	17.02409063	26.08685677	4.35298806
C	15.24619309	26.51226448	2.85502234
C	17.52391939	27.37562981	4.16650668
C	15.70418261	27.81234243	2.64012533
C	16.86249953	28.26486084	3.29908886
H	18.43250398	27.69270826	4.66426268
H	15.16452733	28.48700130	1.98638257
C	12.91347706	6.91705299	3.21581806
C	11.06021435	7.41955706	1.83857163
C	12.82052205	5.56344981	2.89168127
C	10.93148881	6.07821233	1.47837936
C	11.81819276	5.12196268	2.00775396
H	13.49899898	4.84294638	3.33257513
H	10.16881877	5.76762217	0.77450419
C	17.59591047	25.03219043	5.22092846
C	18.73937741	25.22192958	6.00198011
C	19.21895726	24.18438460	6.79657711
H	19.25035101	26.17760300	5.98961795
C	17.40665790	22.83263741	5.99845590
C	18.53989902	22.96620873	6.79422344
H	20.10578503	24.32699962	7.40547438
H	16.84462969	21.90665417	5.96316872
H	18.87435010	22.12852104	7.39636481
C	14.05101272	25.88191711	2.24859755
C	13.20520411	26.54734766	1.35678310
C	12.09756903	25.89096509	0.82734638
H	13.41227017	27.57415552	1.07846575
C	12.72981731	23.95594344	2.09399602
C	11.85510351	24.57005443	1.20332168
H	11.43771305	26.40343844	0.13489195
H	12.58423139	22.93163261	2.41673830
H	11.00535254	24.01698467	0.81840544
C	13.90005628	7.54445374	4.12448046
C	14.89804970	6.82230952	4.78467371
C	15.78993525	7.47942071	5.62765727
H	14.97632264	5.75106310	4.63958726
C	14.65527091	9.52760533	5.11169943
C	15.66567470	8.85841201	5.79490998
H	16.56609116	6.92311609	6.14306311
H	14.51809033	10.59828299	5.20809940
H	16.33560934	9.41456513	6.44143721
C	10.21869155	8.54605779	1.37470119
C	9.14856768	8.38715163	0.48973685
C	8.40210469	9.49404628	0.09535364
H	8.90039673	7.40205463	0.11187131
C	9.81698480	10.84969870	1.47686166
C	8.74347345	10.74945178	0.59776781

H	7.57027981	9.37596001	-0.59145337
H	10.12143910	11.80195210	1.89509352
H	8.19245107	11.64122150	0.31974152
N	13.87175408	23.99305924	5.64453797
N	16.24095974	22.67688626	2.43774032
N	10.94351177	9.93892290	4.93236983
N	13.53797882	10.55120558	1.68702136
N	10.54582919	9.78682725	1.86619421
N	13.78685474	8.90340325	4.29388234
N	13.80410047	24.57996518	2.61247676
N	16.93254789	23.82877776	5.22666933
C	11.69943316	3.68984738	1.64512415
C	10.44256830	3.09901207	1.42753070
C	12.84038048	2.88102659	1.50426525
C	10.33475330	1.75291784	1.08579003
H	9.53847235	3.68885917	1.55006876
C	12.72523575	1.53622693	1.15925823
H	13.82893211	3.31278620	1.63316299
C	11.47197717	0.94399846	0.94698040
H	9.34895356	1.32140617	0.92983365
H	13.62593485	0.93827653	1.04332350
C	17.37474110	29.63891534	3.08450633
C	17.27796966	30.26057553	1.82811768
C	17.97165171	30.36120985	4.13300066
C	17.76367918	31.55166154	1.63005871
H	16.84318573	29.72303489	0.99006407
C	18.45143969	31.65241128	3.92880906
H	18.03296076	29.92302675	5.12525975
C	18.36188628	32.27209038	2.67327624
H	17.68238914	32.00479390	0.64509109
H	18.89513777	32.19249890	4.76176867
C	11.34947110	-0.52131417	0.60329470
H	11.24641939	-1.13122623	1.51076975
H	10.46925984	-0.71463842	-0.01860794
H	12.23406665	-0.88183780	0.06834406
C	18.91315477	33.66018131	2.45066065
H	19.99413647	33.62827727	2.25984014
H	18.44329988	34.14465403	1.58889845
H	18.75961405	34.29668830	3.32866027
N	12.03878226	7.80184619	2.68851213
N	15.91066037	25.69057117	3.69742039
Cl	10.99131039	17.16632194	7.28393306

Cartesian coordinates of DFT-optimized structure of $\mathbf{1}^{3+}$:

Charge = 3; multiplicity=2

O	13.98780292	16.71239904	3.31917269
N	12.50758821	15.77637418	4.83194594
H	11.93917766	15.97837855	5.64524083
C	12.30326071	11.74899077	3.73214413
C	11.59337281	12.22696652	4.86351486
C	11.68436733	13.56724734	5.20703980
H	11.15980821	13.96784548	6.07095630
C	12.47936745	14.44893808	4.42427915
C	13.18826039	13.97388974	3.29034417
H	13.78115783	14.67777819	2.72491576
C	13.09611841	12.62866349	2.95394271
C	13.22992447	16.84169980	4.27646230
N	12.98468426	18.02405942	4.93050113
H	12.32018406	18.00823284	5.69376553
C	14.50450450	21.90159259	4.26921140
C	13.56894002	21.64940904	5.29646984
C	13.08376878	20.35429879	5.49128300
H	12.36192228	20.13580886	6.27536356
C	13.52843214	19.30281735	4.66298955
C	14.46226054	19.54228842	3.63585223
H	14.78145237	18.71415523	3.01907538
C	14.94330563	20.84293556	3.44657742
C	10.81824012	11.18030473	5.55682642
C	10.02967399	11.38056159	6.69129915
C	9.34548004	10.30763048	7.25948227
H	9.95222324	12.37078520	7.12588745
C	10.26075591	8.90450700	5.54665473
C	9.46219130	9.04600545	6.67922274
H	8.73127019	10.45729546	8.14156137
H	10.37953842	7.94195957	5.06215763
H	8.94912908	8.18234035	7.08689084
C	13.76378605	11.96408254	1.81784748
C	14.60426790	12.59432761	0.89792934
C	15.18161039	11.85642222	-0.13362621
H	14.80408640	13.65579325	0.99071433
C	14.06177179	9.91664157	0.71658721
C	14.90764644	10.49322845	-0.22801815
H	15.83580164	12.34100020	-0.85124985
H	13.82131344	8.85984471	0.68238498
H	15.33476958	9.87944623	-1.01299842
C	15.91061005	21.27287932	2.42642788
C	16.51078553	20.43660199	1.47690212
C	17.41174308	20.95884077	0.55523135
H	16.26640380	19.37996525	1.46686082
C	17.08243068	23.10960301	1.55547902
C	17.70543153	22.32361763	0.59241890
H	17.87785769	20.31176326	-0.18145302
H	17.27918820	24.17409110	1.62226209
H	18.40097115	22.77594009	-0.10586145
C	13.21320019	22.85367760	6.06077155
C	12.31097870	22.89912594	7.13050219
C	12.05465985	24.10261873	7.77894456

H	11.81368989	21.98964583	7.44988421
C	13.59446441	25.15843931	6.27921507
C	12.70874425	25.25795850	7.34660162
H	11.35531015	24.13908655	8.60853960
H	14.12445612	26.02920010	5.90854112
H	12.54119340	26.21862598	7.82095462
Ru	12.18363410	9.88068297	3.24608583
Ru	15.18845133	23.72311916	3.98657707
C	17.03020776	26.03430238	4.34084737
C	15.26122257	26.46871139	2.83871315
C	17.54422334	27.31662115	4.14880613
C	15.73158155	27.76318197	2.61703943
C	16.89312598	28.20784268	3.27565424
H	18.45494072	27.62726618	4.64632824
H	15.19974095	28.43963274	1.95906201
C	12.93543119	6.96473747	3.20793349
C	11.06889397	7.44991405	1.85767023
C	12.86680860	5.61365318	2.87010185
C	10.95890220	6.11319200	1.47741229
C	11.86638144	5.16515557	1.98693473
H	13.56148206	4.90198164	3.29837284
H	10.19763628	5.80106638	0.77382599
C	17.59029494	24.97902092	5.21660114
C	18.73677666	25.16183594	5.99404976
C	19.20651270	24.12449227	6.79507102
H	19.25850177	26.11132942	5.97398870
C	17.37827685	22.78777307	6.00938812
C	18.51463149	22.91414727	6.80215512
H	20.09606627	24.26180974	7.40102612
H	16.80744123	21.86706557	5.98219036
H	18.84151825	22.07687858	7.40889483
C	14.06019156	25.84755070	2.23291940
C	13.22640968	26.51649382	1.33315822
C	12.11320559	25.86940905	0.80352113
H	13.44672469	27.53840600	1.04780893
C	12.71703096	23.93697413	2.08696195
C	11.85347714	24.55471665	1.18776004
H	11.46288326	26.38469048	0.10433844
H	12.55660352	22.91696990	2.41577716
H	10.99914365	24.00893435	0.80274385
C	13.91967103	7.59729664	4.11620380
C	14.93646961	6.88760766	4.75650175
C	15.82445110	7.55338842	5.59797339
H	15.03399878	5.82034637	4.59816364
C	14.64700368	9.58511679	5.11784616
C	15.67690934	8.92611818	5.78224376
H	16.61626203	7.00627302	6.09847849
H	14.49581705	10.65135772	5.23011719
H	16.34281758	9.48835631	6.42688161
C	10.20413786	8.56739538	1.41386188
C	9.13179641	8.40357570	0.53572617
C	8.36627072	9.50527087	0.16117663
H	8.89557486	7.42064748	0.14628250
C	9.76943245	10.86420308	1.54963470
C	8.69139579	10.75778924	0.67630782

H	7.53213714	9.38315777	-0.52160766
H	10.05786655	11.81765591	1.97390769
H	8.12639726	11.64509973	0.41416264
N	13.85083682	24.00071861	5.64382729
N	16.21019216	22.61637008	2.45315130
N	10.92222715	9.93225135	4.99250056
N	13.50084089	10.61987882	1.71242055
N	10.51342143	9.80457787	1.91678077
N	13.78491377	8.94844962	4.30380556
N	13.79609735	24.55213369	2.60516526
N	16.91390021	23.78377837	5.23218290
C	11.77181043	3.73890364	1.60393164
C	10.52471428	3.13567225	1.36246843
C	12.92717396	2.95020795	1.46532855
C	10.44073152	1.79402387	1.00061069
H	9.61017386	3.70915537	1.48418123
C	12.83497552	1.61068693	1.09631635
H	13.90831764	3.39315810	1.61039381
C	11.59220460	1.00460239	0.86130608
H	9.46351313	1.35021027	0.82779738
H	13.74498682	1.02769517	0.98016183
C	17.41823566	29.57555960	3.05561244
C	17.32746366	30.19210428	1.79631292
C	18.02106644	30.29602305	4.10201584
C	17.82550783	31.47753281	1.59319431
H	16.88875768	29.65499519	0.96004220
C	18.51190755	31.58201409	3.89276646
H	18.07772413	29.86174014	5.09625474
C	18.42896839	32.19687895	2.63423085
H	17.74964794	31.92710899	0.60629283
H	18.95966062	32.12187744	4.72356656
C	11.49434449	-0.45559534	0.49230487
H	11.35638962	-1.07681612	1.38722739
H	10.64191868	-0.64525139	-0.16800650
H	12.40317292	-0.80309252	-0.00892662
C	18.99234022	33.57905616	2.40676396
H	20.07520404	33.53738382	2.22934362
H	18.53621044	34.05956424	1.53559598
H	18.83321689	34.22356135	3.27786825
N	12.04364227	7.83549567	2.70121501
N	15.91553018	25.64665173	3.68590020

Cartesian coordinates of DFT-optimized structure of $[\mathbf{1} \cdot \text{Br}]^{2+}$:

Charge = 2; multiplicity=2

O	14.10297777	16.74080485	3.11161998
N	12.64330842	15.80266503	4.64867015
H	12.06232916	16.04276519	5.46304118
C	12.37977312	11.73433436	3.62497236
C	11.67531919	12.25889978	4.73268557
C	11.78465504	13.61251989	5.04728005
H	11.25619705	14.04926538	5.89164152
C	12.59947413	14.45714493	4.25792681
C	13.30698369	13.94374563	3.15015874
H	13.91996928	14.62058186	2.57084984
C	13.19086336	12.58431415	2.84185499
C	13.35355128	16.83413526	4.08440188
N	13.10718816	18.02476550	4.77351767
H	12.45017290	17.95710849	5.56810880
C	14.54281831	21.90054212	4.19549751
C	13.61824786	21.61002957	5.23449531
C	13.16110058	20.31387483	5.40144119
H	12.45468319	20.04454250	6.18251570
C	13.61787929	19.28141663	4.53103151
C	14.54278783	19.56657300	3.49017115
H	14.86197463	18.75237141	2.85484346
C	14.99660473	20.86976400	3.33188959
C	10.87826411	11.24794538	5.44222420
C	10.08517505	11.48920940	6.57056048
C	9.37476264	10.44888773	7.15987391
H	10.02958117	12.49191266	6.98004059
C	10.26672381	8.98386830	5.48820446
C	9.46586913	9.16855539	6.60990624
H	8.75928621	10.63389260	8.03483261
H	10.36666735	8.00721993	5.02705698
H	8.93059666	8.32671064	7.03516641
C	13.84888590	11.88286261	1.73023769
C	14.70957492	12.47365366	0.79630995
C	15.27536996	11.70661426	-0.21617781
H	14.92989188	13.53291623	0.87041315
C	14.11245861	9.80804223	0.66545424
C	14.97260813	10.34504982	-0.28591399
H	15.94278291	12.16336852	-0.94054067
H	13.84859565	8.75594367	0.65042373
H	15.38981592	9.70732826	-1.05746340
C	15.94999607	21.34504909	2.31358717
C	16.55036936	20.54471925	1.33783433
C	17.43641163	21.10976345	0.42414624
H	16.32092287	19.48583881	1.29767700
C	17.08341230	23.22469573	1.49236951
C	17.70973930	22.47519310	0.50029516
H	17.90506486	20.49221439	-0.33551197
H	17.26512849	24.28927865	1.58896144
H	18.39230614	22.95858858	-0.18963987
C	13.25059292	22.79109059	6.03580105
C	12.35830138	22.79015226	7.11089130
C	12.09077313	23.97546945	7.79157496

H	11.87740664	21.86551418	7.41005785
C	13.60225136	25.09236270	6.30564975
C	12.72313444	25.14956506	7.38366651
H	11.39853848	23.98015568	8.62751991
H	14.11658058	25.97953322	5.95300280
H	12.54536808	26.09501478	7.88380405
Ru	12.22213609	9.82962753	3.17554962
Ru	15.18757760	23.71003689	3.96323012
C	17.01356551	26.05934728	4.36414308
C	15.23494362	26.51162724	2.88539949
C	17.51958263	27.34798982	4.19628241
C	15.69278921	27.81400654	2.68654092
C	16.85660746	28.25241068	3.34562625
H	18.43231146	27.65279031	4.69310921
H	15.15108633	28.49924763	2.04642917
C	12.92136349	6.93527960	3.23159589
C	11.06963032	7.42352943	1.85132927
C	12.82461793	5.57723509	2.92751795
C	10.93584928	6.07807755	1.50886623
C	11.81991407	5.12657440	2.05093883
H	13.50111643	4.86109815	3.37813534
H	10.17193213	5.76064285	0.80970596
C	17.58655810	24.98831581	5.21305523
C	18.72779785	25.16361043	5.99775283
C	19.20744389	24.10963847	6.77165969
H	19.23716064	26.11976895	6.00633535
C	17.39736390	22.77287763	5.94606153
C	18.53103810	22.89211185	6.74429630
H	20.09329989	24.24112717	7.38402492
H	16.83903047	21.84618535	5.89563845
H	18.86503150	22.04232759	7.32884894
C	14.03434348	25.89375708	2.27435780
C	13.18471257	26.57545105	1.40134193
C	12.07245370	25.92890578	0.86769933
H	13.39073276	27.60648470	1.14003912
C	12.71001063	23.97138483	2.09504908
C	11.83056466	24.60329592	1.22095651
H	11.40894417	26.45448203	0.18910479
H	12.56114465	22.94231622	2.39799245
H	10.97811113	24.05744429	0.83273460
C	13.91171787	7.57240044	4.13042894
C	14.90827076	6.85589248	4.79773147
C	15.80420340	7.52136034	5.63017526
H	14.98285565	5.78273039	4.66686994
C	14.67523824	9.56584437	5.08921474
C	15.68502337	8.90228218	5.77922263
H	16.57950025	6.96927786	6.15120164
H	14.54345327	10.63807119	5.17252098
H	16.35800226	9.46494455	6.41671865
C	10.22937533	8.54596296	1.37341836
C	9.15634801	8.37612251	0.49485614
C	8.41049866	9.47884493	0.08704586
H	8.90452870	7.38623218	0.13262809
C	9.83259415	10.85121268	1.44380871
C	8.75577444	10.74026167	0.56973032

H	7.57602710	9.35217672	-0.59486512
H	10.13842410	11.80945038	1.84657651
H	8.20547762	11.62898634	0.28108314
N	13.86646014	23.95468707	5.64304665
N	16.22866193	22.68883011	2.37853698
N	10.95809002	9.98167296	4.90866251
N	13.55892217	10.53921744	1.64968376
N	10.56015582	9.79244119	1.84537018
N	13.80349715	8.93307046	4.28211490
N	13.78703535	24.58821558	2.61495864
N	16.92597408	23.78635769	5.19653853
C	11.69510481	3.69006775	1.71006977
C	10.43563549	3.10215587	1.50225046
C	12.83317520	2.87445174	1.58257525
C	10.32205241	1.75061168	1.18387533
H	9.53397430	3.69752472	1.61516053
C	12.71212083	1.52513973	1.25998033
H	13.82351873	3.30416960	1.70393156
C	11.45556342	0.93483687	1.05887196
H	9.33456348	1.32058127	1.03567844
H	13.61004149	0.92135609	1.15349865
C	17.37264884	29.62596341	3.14794527
C	17.26102371	30.26811662	1.90309403
C	17.98783231	30.32533470	4.20151161
C	17.75227149	31.55888730	1.72066180
H	16.81309967	29.74758972	1.06138144
C	18.46974133	31.61759015	4.01319461
H	18.06025503	29.87025084	5.18522564
C	18.36700406	32.25822038	2.76888022
H	17.66175694	32.02904472	0.74478839
H	18.92630260	32.14173878	4.84910544
C	11.32845075	-0.53583447	0.74149365
H	11.31592523	-1.13627699	1.66087981
H	10.40175534	-0.75005069	0.19970285
H	12.17035752	-0.88840918	0.13651647
C	18.92175157	33.64694680	2.56285450
H	20.00275915	33.61271945	2.37322333
H	18.45431391	34.14226491	1.70620466
H	18.76951453	34.27321257	3.44826983
N	12.04932881	7.81324842	2.69345737
N	15.90022648	25.68003589	3.70894014
Br	10.96013243	17.26038441	7.21929400

Cartesian coordinates of DFT-optimized structure of $[\mathbf{1}\cdots\text{Cl}]^{2+}$:

Charge = 2; multiplicity=2

O	14.07009051	16.71543154	3.13496024
N	12.62014628	15.77396659	4.68863015
H	12.04775197	16.01545800	5.51515181
C	12.36041688	11.74054399	3.64596308
C	11.65165756	12.25407183	4.76499947
C	11.75879325	13.59660795	5.08578801
H	11.23557231	14.03177988	5.93311473
C	12.57663457	14.45470029	4.29390019
C	13.28681145	13.94555171	3.17241578
H	13.89505418	14.63222053	2.60070554
C	13.17292346	12.59726931	2.85854603
C	13.33535536	16.83014971	4.11679422
N	13.09764593	17.99447555	4.80593330
H	12.45144092	17.92393829	5.60281288
C	14.54655678	21.89738452	4.21433681
C	13.61960197	21.60766235	5.24148182
C	13.15750694	20.30330452	5.41242469
H	12.44478540	20.04763512	6.19285816
C	13.61544285	19.27362434	4.55784352
C	14.54087829	19.55273538	3.52952051
H	14.86872529	18.74026039	2.89583145
C	14.99941419	20.86379953	3.36582038
C	10.85734764	11.23352006	5.47204005
C	10.06670508	11.46804485	6.59984870
C	9.36204630	10.41827134	7.18380733
H	10.00553748	12.46774254	7.01511678
C	10.26129286	8.96766325	5.50226565
C	9.46007310	9.14341725	6.62718853
H	8.74642260	10.59492769	8.06003357
H	10.36598555	7.99415650	5.03627001
H	8.93016728	8.29634365	7.04824550
C	13.83264122	11.90139646	1.73889799
C	14.68764158	12.50028731	0.80953306
C	15.25388155	11.73574282	-0.20734736
H	14.90560365	13.55957285	0.88603450
C	14.09696885	9.83100461	0.67136050
C	14.95494097	10.37555350	-0.28020560
H	15.91860226	12.19635113	-0.93126628
H	13.83665259	8.77833374	0.65368235
H	15.37259199	9.74138278	-1.05414276
C	15.95616512	21.33193116	2.35326277
C	16.56506980	20.52703547	1.38210921
C	17.45594816	21.08353647	0.47092745
H	16.33452039	19.46789250	1.34759275
C	17.09984675	23.20494551	1.52294721
C	17.73123172	22.45102923	0.53992317
H	17.92853028	20.46057319	-0.28230169
H	17.28203083	24.27021657	1.61466596
H	18.41866128	22.92941414	-0.14900974
C	13.24698313	22.78927980	6.03255888
C	12.34677363	22.79561114	7.10491097
C	12.07228711	23.98066348	7.77926826

H	11.86595424	21.87087935	7.40476878
C	13.59045759	25.09471902	6.29958961
C	12.70578536	25.15613305	7.37066346
H	11.37454416	23.98716061	8.61097720
H	14.10564778	25.98163739	5.94669850
H	12.52322567	26.10337297	7.86611159
Ru	12.21221396	9.86506420	3.19362734
Ru	15.20043904	23.73283072	3.97211264
C	17.01402695	26.06137419	4.36800722
C	15.23845307	26.50145376	2.87515707
C	17.51687239	27.35055231	4.19267489
C	15.69736193	27.80286159	2.67053213
C	16.85679844	28.24783065	3.33257075
H	18.42625519	27.66163826	4.69239880
H	15.15864674	28.48354165	2.02257298
C	12.91854446	6.94763107	3.22403548
C	11.06520026	7.43524664	1.85326809
C	12.82715629	5.59048252	2.91552935
C	10.93361240	6.09186367	1.50311180
C	11.82186451	5.14050801	2.03900428
H	13.50696210	4.87545768	3.36217133
H	10.16952194	5.77648181	0.80371646
C	17.58480732	24.99816227	5.22735488
C	18.72483022	25.18232574	6.01382326
C	19.20350613	24.13758787	6.79991654
H	19.23379592	26.13899618	6.01335853
C	17.39636783	22.79113875	5.98249125
C	18.52699164	22.91877482	6.78331614
H	20.08779846	24.27600587	7.41330086
H	16.83702727	21.86415875	5.93772614
H	18.86051852	22.07576694	7.37833177
C	14.04194754	25.87795580	2.26268459
C	13.19613423	26.55408049	1.37980028
C	12.08715774	25.90450234	0.84420232
H	13.40341767	27.58371648	1.11294633
C	12.71918079	23.95520773	2.08816724
C	11.84390929	24.58020924	1.20534238
H	11.42707262	26.42547406	0.15848639
H	12.57153912	22.92762753	2.39867132
H	10.99326898	24.03217455	0.81548803
C	13.90932117	7.58399979	4.12348039
C	14.91036381	6.86975301	4.78403068
C	15.80570844	7.53669865	5.61667324
H	14.98958514	5.79776056	4.64853837
C	14.66632113	9.57817420	5.08808551
C	15.68120086	8.91545944	5.77189543
H	16.58496570	6.98606929	6.13296720
H	14.53235854	10.64901664	5.17776085
H	16.35304250	9.47922345	6.40916999
C	10.22020516	8.55767815	1.38273494
C	9.14762765	8.39063621	0.50491948
C	8.39856725	9.49473612	0.10526944
H	8.89805295	7.40274891	0.13648949
C	9.81790488	10.86224771	1.46908889
C	8.74036305	10.75314110	0.59527820

H	7.56397980	9.37022219	-0.57664358
H	10.11907362	11.81968107	1.87574497
H	8.18808287	11.64257984	0.31366304
N	13.86385130	23.95524688	5.63910983
N	16.23710934	22.67839568	2.41053867
N	10.94366126	9.97353786	4.93125876
N	13.54602358	10.56000527	1.65542070
N	10.54681352	9.80102661	1.86084463
N	13.79663494	8.94168721	4.28214598
N	13.79421454	24.57292453	2.61179756
N	16.92388346	23.79430540	5.21943298
C	11.70059899	3.70615909	1.69242720
C	10.44214469	3.11832043	1.47757637
C	12.84106709	2.89343567	1.56703970
C	10.33196390	1.76781928	1.15512960
H	9.53896766	3.71142226	1.58962590
C	12.72297648	1.54567032	1.23838194
H	13.83044164	3.32381828	1.69306535
C	11.46761066	0.95454562	1.03120395
H	9.34586025	1.33656546	1.00236200
H	13.62193390	0.94358500	1.13250647
C	17.37175702	29.62195368	3.12806604
C	17.27286818	30.25351127	1.87682643
C	17.97344610	30.33344778	4.18120093
C	17.76191035	31.54457951	1.68805889
H	16.83477520	29.72408240	1.03536869
C	18.45536438	31.62511023	3.98637981
H	18.03636972	29.88702364	5.16962745
C	18.36425768	32.25491625	2.73586667
H	17.67983581	32.00588142	0.70706040
H	18.90227409	32.15748017	4.82248709
C	11.34379610	-0.51492210	0.70856521
H	11.32807430	-1.11725016	1.62661005
H	10.41965413	-0.72861887	0.16241364
H	12.18901398	-0.86449560	0.10665887
C	18.91813100	33.64335390	2.52328582
H	20.00027302	33.61069202	2.33958859
H	18.45440271	34.13216296	1.66075880
H	18.75969549	34.27576098	3.40333309
N	12.04353681	7.82202425	2.69312547
N	15.90166716	25.67355039	3.70939345
Cl	11.04176501	17.04947405	7.14764917