

Anion Receptors Based on Highly Fluorinated Aromatic Scaffolds

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Table S1. Cartesian coordinates (in Å) of **R₁...X** complexes.

R₁...N₂				R₁...O₃			
6	-1.262484000	-0.008182000	-1.063236000	6	-1.205897000	-0.212055000	-1.352816000
6	-1.479497000	-1.178898000	-0.344997000	6	-1.279253000	-1.319009000	-0.516038000
6	-2.245004000	0.971978000	-0.974898000	6	-2.203426000	0.749433000	-1.217002000
6	-2.614815000	-1.381547000	0.423895000	6	-2.270590000	-1.455989000	0.443551000
6	-3.396350000	0.797871000	-0.217751000	6	-3.219462000	0.633194000	-0.277411000
6	-3.581079000	-0.385767000	0.483875000	6	-3.245262000	-0.467874000	0.565058000
6	-0.018472000	0.177930000	-1.891506000	6	0.000910000	-0.011026000	-2.233790000
1	-0.118395000	1.100770000	-2.466806000	1	-0.159641000	0.852023000	-2.882287000
1	0.063843000	-0.641656000	-2.608587000	1	0.161394000	-0.880600000	-2.873495000
6	1.240786000	0.225660000	-1.067754000	6	1.207690000	0.198564000	-1.354684000
6	2.205174000	-0.774287000	-1.135525000	6	2.204973000	-0.761813000	-1.209619000
6	1.481899000	1.273453000	-0.185348000	6	1.280754000	1.313099000	-0.527868000
6	3.355872000	-0.742267000	-0.359267000	6	3.219955000	-0.637643000	-0.269837000
6	2.620418000	1.332897000	0.604211000	6	2.271431000	1.458351000	0.431186000
6	3.561866000	0.315329000	0.515457000	6	3.245454000	0.470932000	0.562577000
7	-0.366169000	-0.103194000	2.458847000	9	4.197159000	0.599798000	1.474819000
7	0.587503000	-0.620033000	2.262072000	9	4.151592000	-1.577554000	-0.153652000
9	4.655204000	0.355785000	1.266515000	9	2.298538000	2.520333000	1.228403000
9	4.259732000	-1.712950000	-0.446137000	9	0.352746000	2.267753000	-0.631159000
9	2.810865000	2.344449000	1.446034000	9	2.196274000	-1.850395000	-1.980780000
9	0.576656000	2.253927000	-0.079343000	9	-2.193952000	1.830894000	-1.998254000
9	2.039517000	-1.804779000	-1.969290000	9	-4.151537000	1.573823000	-0.170667000
9	-2.099695000	2.118949000	-1.643994000	9	-4.197329000	-0.587962000	1.478149000
9	-4.321372000	1.751143000	-0.165075000	9	-2.297112000	-2.509832000	1.251590000
9	-4.674805000	-0.563478000	1.213797000	9	-0.350247000	-2.273768000	-0.609297000
9	-2.772978000	-2.505259000	1.117233000	8	-0.852362000	0.686791000	1.794773000
9	-0.551421000	-2.142404000	-0.372404000	8	-0.003306000	0.017956000	2.463961000
				8	0.843093000	-0.662023000	1.802962000
R₁...H₂O				R₁...H₂O₂			
6	-1.250254000	-0.075397000	-1.065694000	6	-1.240743000	-0.154841000	-1.190701000
6	-1.412308000	-1.200590000	-0.267817000	6	-1.384922000	-1.255275000	-0.353805000
6	-2.259862000	0.879047000	-1.013911000	6	-2.244346000	0.805142000	-1.141785000
6	-2.513731000	-1.379296000	0.551644000	6	-2.456687000	-1.392331000	0.511635000
6	-3.380729000	0.726031000	-0.209516000	6	-3.337865000	0.689204000	-0.293890000
6	-3.504502000	-0.408810000	0.580725000	6	-3.439562000	-0.413223000	0.542514000
6	-0.008664000	0.116985000	-1.895771000	6	-0.010082000	0.006018000	-2.043815000
1	-0.124760000	1.022409000	-2.495181000	1	-0.136440000	0.878950000	-2.687430000
1	0.104627000	-0.716130000	-2.592857000	1	0.111704000	-0.863196000	-2.693386000
6	1.236492000	0.215757000	-1.054651000	6	1.225693000	0.160791000	-1.197147000
6	2.238652000	-0.746113000	-1.105211000	6	2.226324000	-0.802824000	-1.156953000
6	1.408298000	1.252973000	-0.146266000	6	1.375385000	1.256295000	-0.355122000
6	3.362839000	-0.685081000	-0.293360000	6	3.323732000	-0.693932000	-0.313753000
6	2.517148000	1.341444000	0.678707000	6	2.451764000	1.386440000	0.505534000
6	3.499823000	0.364620000	0.604515000	6	3.431373000	0.404040000	0.527908000
9	4.565817000	0.429707000	1.396062000	8	-0.386184000	0.579275000	2.053838000
9	4.305130000	-1.622618000	-0.367190000	1	0.037691000	1.212286000	2.650969000
9	2.629357000	2.332224000	1.561278000	8	0.507398000	-0.556071000	2.176937000
9	0.457434000	2.187447000	-0.035191000	1	-0.059699000	-1.188271000	2.641752000
9	2.133029000	-1.774651000	-1.953963000	9	4.466463000	0.513506000	1.353816000

9	-2.164149000	1.989492000	-1.753243000	9	4.263250000	-1.636462000	-0.299046000
9	-4.331405000	1.657244000	-0.186194000	9	2.536382000	2.431543000	1.331365000
9	-4.564836000	-0.560663000	1.367542000	9	0.447130000	2.219151000	-0.362594000
9	-2.607183000	-2.452274000	1.335307000	9	2.144943000	-1.879639000	-1.946312000
9	-0.456786000	-2.138937000	-0.255862000	9	-2.169776000	1.886285000	-1.925172000
8	0.062060000	-0.283088000	2.179452000	9	-4.279581000	1.629092000	-0.270922000
1	0.277937000	-1.147202000	2.540826000	9	-4.470816000	-0.529702000	1.372286000
1	-0.051167000	0.273472000	2.954322000	9	-2.535006000	-2.441816000	1.332991000
				9	-0.452252000	-2.214004000	-0.364391000
R_l...F⁻				R_l...Cl⁻			
6	-1.234993000	0.191437000	1.055900000	6	-1.237174000	0.130572000	1.210442000
6	-1.315596000	1.220711000	0.124091000	6	-1.464680000	1.286487000	0.474627000
6	-2.265774000	-0.733781000	1.063723000	6	-2.128798000	-0.916842000	1.020806000
6	-2.399193000	1.356199000	-0.727511000	6	-2.518299000	1.408552000	-0.412720000
6	-3.347646000	-0.643074000	0.202780000	6	-3.186955000	-0.828646000	0.130924000
6	-3.407622000	0.409766000	-0.698099000	6	-3.379295000	0.339216000	-0.589822000
6	0.001757000	0.024339000	1.897426000	6	-0.000068000	-0.000236000	2.062030000
1	-0.139314000	-0.836367000	2.556440000	1	-0.102454000	-0.876352000	2.706000000
1	0.144751000	0.899154000	2.536912000	1	0.102287000	0.875883000	2.705995000
6	1.234985000	-0.162257000	1.054704000	6	1.237079000	-0.131016000	1.210495000
6	2.273224000	0.754760000	1.047201000	6	2.128911000	0.916279000	1.021241000
6	1.304442000	-1.204799000	0.136225000	6	1.464349000	-1.286704000	0.474256000
6	3.354828000	0.640779000	0.188911000	6	3.187086000	0.828166000	0.131366000
6	2.389682000	-1.365035000	-0.709803000	6	2.517917000	-1.408666000	-0.413147000
6	3.406286000	-0.427866000	-0.694403000	6	3.379171000	-0.339462000	-0.589813000
9	4.449293000	-0.549861000	-1.527980000	9	4.393701000	-0.430891000	-1.452138000
9	4.356128000	1.538138000	0.218936000	9	4.033204000	1.854874000	-0.024206000
9	2.434671000	-2.381012000	-1.576817000	9	2.691640000	-2.526354000	-1.115706000
9	0.371291000	-2.159168000	0.166166000	9	0.628427000	-2.320995000	0.617262000
9	2.248589000	1.805584000	1.894622000	9	1.992151000	2.054672000	1.724030000
9	-2.233403000	-1.770391000	1.927513000	9	-1.991886000	-2.055410000	1.723281000
9	-4.340315000	-1.548860000	0.245209000	9	-4.032887000	-1.855463000	-0.025006000
9	-4.449996000	0.509617000	-1.534977000	9	-4.393859000	0.430743000	-1.452096000
9	-2.452840000	2.357679000	-1.610491000	9	-2.692330000	2.526501000	-1.114776000
9	-0.382826000	2.175660000	0.130938000	9	-0.629089000	2.320963000	0.618087000
9	0.002552000	-0.025148000	-1.526479000	17	0.000767000	0.001559000	-2.07557000
R_l...BF₄⁻				R_l...NO₃⁻			
6	1.249456000	-1.527481000	0.050403000	6	-1.131930000	-0.007304000	1.412176000
6	1.409774000	-0.920701000	-1.190938000	6	-1.343982000	1.218003000	0.785985000
6	2.180287000	-1.208316000	1.029889000	6	-2.057552000	-1.010349000	1.157299000
6	2.412232000	0.000490000	-1.442539000	6	-2.405479000	1.438120000	-0.074708000
6	3.199842000	-0.297873000	0.804651000	6	-3.123603000	-0.822913000	0.291742000
6	3.304547000	0.320818000	-0.431114000	6	-3.289599000	0.401091000	-0.335873000
6	0.033110000	-2.373716000	0.333674000	6	0.119501000	-0.240076000	2.220655000
1	0.161763000	-2.875846000	1.294377000	1	0.024176000	-1.181552000	2.765090000
1	-0.082298000	-3.143218000	-0.432544000	1	0.247956000	0.559007000	2.954070000
6	-1.201270000	-1.508070000	0.356194000	6	1.324684000	-0.281628000	1.316445000
6	-2.096403000	-1.464533000	-0.703554000	6	2.196346000	0.791954000	1.188751000
6	-1.415905000	-0.613780000	1.399827000	6	1.532010000	-1.368395000	0.474569000
6	-3.132438000	-0.546534000	-0.750603000	6	3.210389000	0.806108000	0.246757000
6	-2.436364000	0.321686000	1.376710000	6	2.535534000	-1.380065000	-0.478402000
6	-3.290503000	0.361078000	0.284622000	6	3.368028000	-0.279809000	-0.599564000

9	-4.279415000	1.252212000	0.242191000	9	4.335933000	-0.271107000	-1.520016000
9	-3.980934000	-0.527741000	-1.785223000	9	4.039204000	1.853235000	0.148227000
9	-2.608227000	1.164988000	2.390170000	9	2.703069000	-2.432249000	-1.280897000
9	-0.614297000	-0.665388000	2.468050000	9	0.763220000	-2.451765000	0.613969000
9	-1.978712000	-2.333456000	-1.722335000	9	2.084585000	1.852229000	2.007652000
9	2.115772000	-1.791234000	2.239083000	9	-1.937935000	-2.207551000	1.754917000
9	4.081601000	-0.010415000	1.769014000	9	-3.990960000	-1.813724000	0.058725000
9	4.277954000	1.202406000	-0.654708000	9	-4.315169000	0.593141000	-1.162003000
9	2.527749000	0.571158000	-2.638053000	9	-2.588154000	2.626498000	-0.642567000
9	0.571384000	-1.238804000	-2.180609000	9	-0.504042000	2.228181000	1.034883000
9	0.956624000	2.871335000	-0.754734000	8	-0.415777000	-1.020213000	-1.544671000
5	-0.058537000	2.075095000	-0.215604000	7	-0.360448000	0.169940000	-1.960405000
9	-1.159497000	2.837138000	0.193469000	8	-1.215840000	0.595637000	-2.765806000
9	0.455091000	1.358870000	0.897329000	8	0.548762000	0.931146000	-1.532939000
9	-0.485646000	1.129508000	-1.184437000				
R_{I...}ClO⁻				R_{I...}ClO₂⁻			
6	-1.124356000	0.757657000	0.978838000	6	-0.974896000	1.055957000	0.987630000
6	-1.316660000	1.310224000	-0.284623000	6	-1.182995000	1.468861000	-0.321842000
6	-2.140656000	-0.037699000	1.479796000	6	-1.985939000	0.311489000	1.580518000
6	-2.480285000	1.102758000	-1.003825000	6	-2.343952000	1.165481000	-1.014016000
6	-3.321862000	-0.259145000	0.783673000	6	-3.148103000	-0.025409000	0.905781000
6	-3.486080000	0.312442000	-0.465368000	6	-3.325701000	0.405233000	-0.397180000
6	0.151693000	1.000620000	1.738317000	6	0.322846000	1.352377000	1.690538000
1	0.056987000	0.539888000	2.725271000	1	0.235546000	1.036382000	2.732953000
1	0.281826000	2.074328000	1.899080000	1	0.511614000	2.428873000	1.693519000
6	1.376403000	0.472354000	1.043967000	6	1.497661000	0.663785000	1.048038000
6	2.384717000	1.309076000	0.587749000	6	2.492466000	1.366638000	0.380810000
6	1.509064000	-0.888216000	0.778992000	6	1.596880000	-0.722653000	1.049249000
6	3.499020000	0.828931000	-0.080466000	6	3.537869000	0.728167000	-0.266360000
6	2.623652000	-1.398220000	0.128065000	6	2.626988000	-1.388196000	0.404941000
6	3.612589000	-0.535461000	-0.310244000	6	3.601187000	-0.656860000	-0.254464000
9	4.682507000	-1.010606000	-0.962379000	9	4.602530000	-1.282352000	-0.883225000
9	4.470136000	1.663381000	-0.489406000	9	4.489427000	1.435145000	-0.893226000
9	2.732953000	-2.708120000	-0.106192000	9	2.690305000	-2.719285000	0.411907000
9	0.621270000	-1.740780000	1.300170000	9	0.683129000	-1.439475000	1.699801000
9	2.302507000	2.638468000	0.801388000	9	2.465116000	2.712623000	0.352940000
9	-2.010365000	-0.615320000	2.688905000	9	-1.841295000	-0.127642000	2.845063000
9	-4.290007000	-1.027102000	1.305034000	9	-4.086970000	-0.765714000	1.498741000
9	-4.609141000	0.097854000	-1.157982000	9	-4.438686000	0.092906000	-1.060116000
9	-2.643296000	1.647353000	-2.211839000	9	-2.525012000	1.598091000	-2.268194000
9	-0.391182000	2.134906000	-0.782797000	9	-0.254262000	2.222813000	-0.928060000
17	-1.038919000	-1.783500000	-1.77082200	17	-1.078585000	-1.647591000	-1.81113800
8	0.226365000	-0.733369000	-1.279215000	8	0.235519000	-0.924098000	-1.212067000
				8	-2.079972000	-2.244579000	-0.710391000
R_{I...}ClO₃⁻				R_{I...}ClO₄⁻			
6	1.292175000	0.617300000	1.294154000	6	-1.222231000	-1.635177000	0.109748000
6	1.540694000	-0.748356000	1.207018000	6	-1.436697000	-0.923940000	1.285143000
6	2.170935000	1.456593000	0.623832000	6	-2.112378000	-1.407411000	-0.932240000
6	2.602569000	-1.270396000	0.486096000	6	-2.458898000	0.000157000	1.418784000
6	3.231692000	0.965949000	-0.119313000	6	-3.145343000	-0.489803000	-0.827997000
6	3.443051000	-0.401370000	-0.193322000	6	-3.309350000	0.226951000	0.346965000
6	0.073704000	1.142558000	2.010173000	6	0.008239000	-2.494753000	-0.040355000

1	0.186086000	2.219386000	2.151387000	1	-0.095762000	-3.119865000	-0.929575000
1	-0.003939000	0.683965000	2.998517000	1	0.114430000	-3.154391000	0.823358000
6	-1.185813000	0.853138000	1.235240000	6	1.235897000	-1.626294000	-0.157580000
6	-2.058729000	-0.164524000	1.598865000	6	2.119312000	-1.425774000	0.895575000
6	-1.478829000	1.545308000	0.062426000	6	1.454036000	-0.880961000	-1.310945000
6	-3.153696000	-0.509080000	0.820768000	6	3.148943000	-0.501466000	0.824048000
6	-2.561232000	1.217490000	-0.737450000	6	2.473457000	0.050648000	-1.411865000
6	-3.394901000	0.175220000	-0.360235000	6	3.316732000	0.249675000	-0.328853000
9	-4.428687000	-0.160910000	-1.124085000	9	4.301461000	1.142756000	-0.403876000
9	-3.976638000	-1.491888000	1.203069000	9	3.976746000	-0.325204000	1.859816000
9	-2.792574000	1.876449000	-1.867434000	9	2.650250000	0.747635000	-2.531021000
9	-0.696741000	2.562085000	-0.303376000	9	0.654056000	-1.069520000	-2.364577000
9	-1.868394000	-0.837921000	2.745927000	9	1.992492000	-2.139351000	2.026371000
9	2.012797000	2.787688000	0.692528000	9	-1.988072000	-2.085762000	-2.084859000
9	4.061656000	1.801914000	-0.750818000	9	-3.979930000	-0.287695000	-1.853514000
9	4.473572000	-0.877578000	-0.890367000	9	-4.298581000	1.111357000	0.455061000
9	2.842204000	-2.576830000	0.469352000	9	-2.631425000	0.663971000	2.558133000
9	0.727117000	-1.601435000	1.847548000	9	-0.628630000	-1.136106000	2.328110000
8	0.754342000	-2.225252000	-1.832737000	8	-1.156526000	2.890807000	0.516059000
17	-0.236284000	-1.145899000	-1.43102000	17	-0.017925000	2.088526000	0.01993400
8	0.420121000	0.218191000	-1.691969000	8	1.079501000	2.962683000	-0.445019000
8	-1.484945000	-1.247466000	-2.299441000	8	-0.478612000	1.226998000	-1.105434000
				8	0.483190000	1.209445000	1.114139000
R_{1...}SO₄²⁻							
6	1.233071000	-1.583101000	0.083091000				
6	1.391159000	-0.995425000	-1.170129000				
6	2.150061000	-1.232417000	1.062973000				
6	2.396918000	-0.078740000	-1.431231000				
6	3.160774000	-0.320168000	0.830426000				
6	3.266770000	0.277409000	-0.416573000				
6	0.011996000	-2.417023000	0.384351000				
1	0.143458000	-2.901963000	1.354689000				
1	-0.108667000	-3.202713000	-0.366452000				
6	-1.222376000	-1.550852000	0.391667000				
6	-2.096155000	-1.506306000	-0.684932000				
6	-1.434141000	-0.631800000	1.417690000				
6	-3.106765000	-0.568908000	-0.771340000				
6	-2.444835000	0.315249000	1.359427000				
6	-3.262104000	0.362795000	0.243715000				
9	-4.251168000	1.261471000	0.170246000				
9	-3.947406000	-0.554927000	-1.826403000				
9	-2.657156000	1.146686000	2.381252000				
9	-0.724752000	-0.751643000	2.549708000				
9	-1.981142000	-2.405752000	-1.690429000				
9	2.077210000	-1.793893000	2.292347000				
9	4.044449000	-0.008196000	1.800407000				
9	4.255890000	1.148441000	-0.651821000				
9	2.554200000	0.431187000	-2.654030000				
9	0.628292000	-1.423912000	-2.185756000				
8	1.167501000	2.723125000	-0.737696000				
16	-0.005601000	1.943477000	-0.22066000				
8	-1.179082000	2.824962000	0.092342000				
8	0.415350000	1.187975000	1.032043000				

8	-0.428416000	0.906389000	-1.251959000	
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Table S2. Cartesian coordinates (in Å) of **R_{II}...X** complexes.

R _{II} ...N ₂				R _{II} ...O ₃			
6	-4.506948000	1.849282000	-0.474740000	6	-4.359977000	1.947403000	-0.423167000
6	-3.304394000	2.052061000	0.189297000	6	-3.219141000	2.082241000	0.357110000
6	-5.085016000	0.587245000	-0.485229000	6	-4.965109000	0.704580000	-0.554579000
6	-2.700533000	0.985943000	0.837029000	6	-2.698383000	0.965902000	0.990904000
6	-4.448875000	-0.463116000	0.163883000	6	-4.415230000	-0.396694000	0.088283000
6	-3.244999000	-0.293902000	0.838553000	6	-3.269280000	-0.296771000	0.868904000
6	4.530867000	1.853590000	-0.489303000	6	4.405908000	1.865412000	-0.425916000
6	5.108638000	0.591323000	-0.509451000	6	5.004197000	0.612490000	-0.404523000
6	3.331330000	2.054643000	0.180924000	6	3.188637000	2.059284000	0.211222000
6	4.474079000	-0.462353000	0.135324000	6	4.375161000	-0.439429000	0.251936000
6	2.730095000	0.985698000	0.826209000	6	2.583910000	0.987812000	0.858211000
6	3.273383000	-0.294911000	0.816418000	6	3.158003000	-0.280571000	0.901342000
6	0.006165000	-2.530604000	-1.114594000	6	-0.032805000	-2.648634000	-1.012533000
6	-1.183217000	-2.262224000	-0.454141000	6	-1.236217000	-2.383651000	-0.380945000
6	1.199959000	-2.264019000	-0.462075000	6	1.147642000	-2.328969000	-0.354012000
6	-1.217072000	-1.759180000	0.841322000	6	-1.299431000	-1.829666000	0.893182000
6	1.243337000	-1.757129000	0.831947000	6	1.162113000	-1.785723000	0.926112000
6	0.015273000	-1.532903000	1.447496000	6	-0.079178000	-1.563609000	1.513378000
6	-2.528962000	-1.438444000	1.508282000	6	-2.627707000	-1.495696000	1.519298000
1	-3.179608000	-2.315447000	1.493946000	1	-3.302421000	-2.349179000	1.427742000
1	-2.339952000	-1.193681000	2.555390000	1	-2.481469000	-1.305208000	2.584319000
6	2.561055000	-1.440149000	1.489230000	6	2.460521000	-1.421353000	1.595014000
1	2.381131000	-1.197397000	2.538423000	1	2.255958000	-1.151696000	2.632998000
1	3.209405000	-2.318716000	1.467072000	1	3.129356000	-2.284389000	1.611337000
9	5.052641000	-1.666411000	0.091644000	9	4.980078000	-1.630108000	0.251056000
9	6.260472000	0.402357000	-1.147358000	9	6.170986000	0.428926000	-1.011256000
9	-2.334582000	-2.485220000	-1.095875000	9	-2.370040000	-2.642505000	-1.034698000
9	-5.029811000	-1.665903000	0.129828000	9	-5.026004000	-1.577616000	-0.053904000
9	-6.239580000	0.395207000	-1.116210000	9	-6.064643000	0.578058000	-1.292780000
9	-2.734775000	3.254077000	0.188839000	9	-2.632481000	3.267824000	0.480028000
9	-1.537421000	1.200726000	1.461302000	9	-1.594882000	1.110380000	1.729384000
9	0.019489000	-1.069565000	2.709763000	9	-0.103507000	-1.074402000	2.762658000
9	2.347914000	-2.500617000	-1.106445000	9	2.306050000	-2.543035000	-0.982825000
9	1.581896000	1.199511000	1.475625000	9	1.412204000	1.189852000	1.460832000
9	2.769131000	3.259073000	0.196901000	9	2.603066000	3.247589000	0.184521000
9	5.124070000	2.866350000	-1.109449000	9	4.996361000	2.872128000	-1.056082000
9	-5.101086000	2.858788000	-1.098566000	9	-4.872882000	3.004898000	-1.041312000
9	0.001455000	-3.017462000	-2.353000000	9	-0.005319000	-3.155321000	-2.241001000
7	0.258904000	1.122739000	-1.249742000	8	1.302357000	0.939714000	-1.636538000
7	-0.718086000	0.731822000	-1.578273000	8	0.292651000	0.176116000	-1.729290000
				8	-0.781772000	0.543457000	-1.154586000
R _{II} ...H ₂ O				R _{II} ...H ₂ O ₂			
6	-4.437180000	1.859398000	-0.507950000	6	-4.336612000	1.872863000	-0.341165000
6	-3.238858000	2.029091000	0.171402000	6	-3.180932000	2.001863000	0.415425000
6	-5.041926000	0.610319000	-0.535353000	6	-4.940282000	0.629716000	-0.465141000

6	-2.664791000	0.945497000	0.814788000	6	-2.643839000	0.885381000	1.032998000
6	-4.434207000	-0.459006000	0.109903000	6	-4.370103000	-0.474550000	0.155119000
6	-3.233920000	-0.322295000	0.798372000	6	-3.207982000	-0.379501000	0.911182000
6	4.430949000	1.863081000	-0.516771000	6	4.511274000	1.838281000	-0.489469000
6	5.040247000	0.616106000	-0.535780000	6	5.124182000	0.593775000	-0.449374000
6	3.232974000	2.033962000	0.163218000	6	3.285159000	2.022551000	0.136241000
6	4.436561000	-0.450875000	0.117105000	6	4.497457000	-0.457244000	0.207506000
6	2.664199000	0.953528000	0.816604000	6	2.692915000	0.957555000	0.796206000
6	3.236757000	-0.313023000	0.805955000	6	3.270313000	-0.306687000	0.843242000
6	0.009072000	-2.484846000	-1.188388000	6	0.036664000	-2.402357000	-1.184665000
6	-1.183329000	-2.247414000	-0.524049000	6	-1.158079000	-2.238373000	-0.504299000
6	1.197639000	-2.243118000	-0.518618000	6	1.223623000	-2.167576000	-0.511339000
6	-1.225461000	-1.799408000	0.790423000	6	-1.204558000	-1.847877000	0.828505000
6	1.232658000	-1.794231000	0.795904000	6	1.254684000	-1.778600000	0.822069000
6	0.001772000	-1.595858000	1.411638000	6	0.021494000	-1.636701000	1.449682000
6	-2.541285000	-1.489346000	1.453084000	6	-2.525145000	-1.584799000	1.504479000
1	-3.200785000	-2.358726000	1.409918000	1	-3.182378000	-2.450580000	1.400701000
1	-2.363847000	-1.269892000	2.507811000	1	-2.355573000	-1.430170000	2.571706000
6	2.544556000	-1.478355000	1.464182000	6	2.558316000	-1.458091000	1.504275000
1	2.360977000	-1.253933000	2.516754000	1	2.356217000	-1.216808000	2.549755000
1	3.206154000	-2.346517000	1.428917000	1	3.216791000	-2.329594000	1.496924000
9	5.044071000	-1.639925000	0.069997000	9	5.106496000	-1.646643000	0.209724000
9	6.190723000	0.453410000	-1.182964000	9	6.298481000	0.417014000	-1.047876000
9	-2.332672000	-2.450128000	-1.179064000	9	-2.300716000	-2.446537000	-1.166189000
9	-5.038219000	-1.649509000	0.056093000	9	-4.976057000	-1.656932000	0.008080000
9	-6.192557000	0.448305000	-1.182290000	9	-6.054435000	0.503412000	-1.181986000
9	-2.645037000	3.222336000	0.193398000	9	-2.573764000	3.185733000	0.514227000
9	-1.510195000	1.136780000	1.469749000	9	-1.524378000	1.037276000	1.751061000
9	-0.002230000	-1.175616000	2.691583000	9	0.017713000	-1.262241000	2.743431000
9	2.350354000	-2.442637000	-1.168797000	9	2.375700000	-2.304262000	-1.181399000
9	1.514352000	1.145911000	1.477336000	9	1.517660000	1.163494000	1.403583000
9	2.636085000	3.225612000	0.177727000	9	2.686474000	3.212306000	0.098280000
9	4.991235000	2.888992000	-1.147264000	9	5.094945000	2.848866000	-1.122804000
9	-5.001848000	2.887896000	-1.130055000	9	-4.859807000	2.933185000	-0.947382000
9	0.012769000	-2.915799000	-2.447510000	9	0.041922000	-2.742199000	-2.474722000
8	-0.031061000	1.243518000	-1.056725000	8	-0.169954000	0.771738000	-1.005421000
1	-0.008960000	1.898723000	-1.758308000	1	-0.249105000	1.682195000	-0.682813000
1	-0.055094000	1.762345000	-0.246754000	8	-1.328557000	0.676791000	-1.872937000
				1	-0.901261000	0.556700000	-2.732535000
R_{II}...F⁻				R_{II}...Cl⁻			
6	-3.077094000	2.220767000	-0.758553000	6	-3.825727000	2.015846000	-0.616194000
6	-2.311624000	2.205510000	0.391874000	6	-2.817964000	2.108863000	0.329627000
6	-3.723673000	1.066046000	-1.176027000	6	-4.460071000	0.802064000	-0.834931000
6	-2.170165000	1.023846000	1.104187000	6	-2.442629000	0.974977000	1.032606000
6	-3.573265000	-0.098000000	-0.441322000	6	-4.069496000	-0.312897000	-0.110974000
6	-2.792589000	-0.156628000	0.707593000	6	-3.047611000	-0.261380000	0.829185000
6	3.049187000	2.243677000	-0.763323000	6	3.824877000	2.016425000	-0.616596000
6	3.709025000	1.095752000	-1.179044000	6	4.459977000	0.802930000	-0.834787000
6	2.286038000	2.222266000	0.388474000	6	2.816875000	2.109211000	0.328991000
6	3.574313000	-0.068285000	-0.441380000	6	4.069938000	-0.311988000	-0.110494000
6	2.161674000	1.041006000	1.104564000	6	2.442128000	0.975366000	1.032360000
6	2.796777000	-0.132954000	0.709386000	6	3.047877000	-0.260693000	0.829492000

6	0.019826000	-3.307507000	-0.766004000	6	0.000704000	-2.830917000	-0.960045000
6	-1.175414000	-2.881522000	-0.210874000	6	-1.186856000	-2.520971000	-0.325343000
6	1.209930000	-2.872135000	-0.207456000	6	1.188053000	-2.520436000	-0.325221000
6	-1.219695000	-2.074664000	0.916461000	6	-1.228305000	-1.951548000	0.940007000
6	1.244443000	-2.065213000	0.920299000	6	1.229094000	-1.951144000	0.940200000
6	0.010227000	-1.730081000	1.465129000	6	0.000310000	-1.707221000	1.541928000
6	-2.508177000	-1.463335000	1.410656000	6	-2.536903000	-1.495158000	1.532753000
1	-3.334683000	-2.156242000	1.240632000	1	-3.285990000	-2.286188000	1.452295000
1	-2.432867000	-1.286903000	2.485769000	1	-2.391534000	-1.282388000	2.593510000
6	2.526382000	-1.440904000	1.415456000	6	2.537472000	-1.494505000	1.533192000
1	2.448211000	-1.262715000	2.490053000	1	2.391877000	-1.281647000	2.593896000
1	3.360071000	-2.125619000	1.247413000	1	3.286752000	-2.285366000	1.452912000
9	4.244535000	-1.158418000	-0.864518000	9	4.738408000	-1.459130000	-0.322251000
9	4.488779000	1.132736000	-2.272474000	9	5.460321000	0.723700000	-1.722409000
9	-2.317104000	-3.284380000	-0.793907000	9	-2.336214000	-2.766067000	-0.969846000
9	-4.231911000	-1.194946000	-0.865335000	9	-4.737272000	-1.460337000	-0.323290000
9	-4.506411000	1.095867000	-2.267614000	9	-5.460229000	0.722564000	-1.722741000
9	-1.685745000	3.313756000	0.789829000	9	-2.231307000	3.279440000	0.560503000
9	-1.506768000	1.070125000	2.257509000	9	-1.500572000	1.090536000	1.966992000
9	0.005747000	-1.058855000	2.626846000	9	0.000137000	-1.189626000	2.789542000
9	2.356733000	-3.265419000	-0.787024000	9	2.337617000	-2.764894000	-0.969609000
9	1.499303000	1.080832000	2.258730000	9	1.499860000	1.090645000	1.966569000
9	1.648427000	3.323802000	0.785642000	9	2.229506000	3.279523000	0.559325000
9	3.169341000	3.371500000	-1.474334000	9	4.204696000	3.097205000	-1.302710000
9	-3.211490000	3.348932000	-1.466623000	9	-4.206000000	3.096661000	-1.302000000
9	0.024492000	-4.123401000	-1.833011000	9	0.000888000	-3.380843000	-2.177159000
9	-0.006537000	0.555162000	0.016901000	17	-0.000594000	0.692956000	-1.06972800
R_{II...}BF₄⁻				R_{II...}NO₃⁻			
6	-3.780650000	1.959736000	-0.308002000	6	-3.817082000	2.006289000	-0.546031000
6	-2.805231000	1.966705000	0.677742000	6	-2.818411000	2.103663000	0.409716000
6	-4.401415000	0.770670000	-0.656951000	6	-4.447352000	0.791788000	-0.769805000
6	-2.454440000	0.775479000	1.291669000	6	-2.445982000	0.967955000	1.110454000
6	-4.024841000	-0.407317000	-0.030344000	6	-4.064176000	-0.322064000	-0.041812000
6	-3.033350000	-0.440883000	0.943119000	6	-3.047316000	-0.269021000	0.903370000
6	3.582768000	2.039320000	-0.303455000	6	3.811846000	2.004458000	-0.547960000
6	4.289616000	0.887577000	-0.615108000	6	4.437157000	0.788091000	-0.775150000
6	2.617801000	2.008803000	0.691464000	6	2.822772000	2.105876000	0.417262000
6	4.003363000	-0.295051000	0.049902000	6	4.056659000	-0.323886000	-0.042968000
6	2.354657000	0.813446000	1.338248000	6	2.452178000	0.971876000	1.121662000
6	3.013317000	-0.370497000	1.022646000	6	3.046620000	-0.267676000	0.909345000
6	0.066094000	-2.833269000	-0.999686000	6	-0.000013000	-2.885116000	-0.850129000
6	-1.133808000	-2.575660000	-0.365032000	6	-1.188726000	-2.563611000	-0.222534000
6	1.241113000	-2.577698000	-0.316013000	6	1.187727000	-2.561565000	-0.221738000
6	-1.201675000	-2.118686000	0.946084000	6	-1.230914000	-1.963776000	1.030542000
6	1.256395000	-2.110631000	0.991682000	6	1.228290000	-1.961471000	1.031554000
6	0.014329000	-1.926182000	1.591925000	6	-0.001745000	-1.703460000	1.627661000
6	-2.529434000	-1.729255000	1.546559000	6	-2.541664000	-1.501272000	1.613659000
1	-3.267785000	-2.515233000	1.373244000	1	-3.292482000	-2.292378000	1.534713000
1	-2.414288000	-1.612798000	2.625771000	1	-2.406573000	-1.288044000	2.677145000
6	2.556140000	-1.677081000	1.625584000	6	2.538462000	-1.500138000	1.617688000
1	2.413575000	-1.563644000	2.701843000	1	2.401503000	-1.288435000	2.681204000
1	3.326660000	-2.434489000	1.467883000	1	3.288552000	-2.292000000	1.538986000

9	4.725486000	-1.383572000	-0.265267000	9	4.715360000	-1.473926000	-0.264190000
9	5.246193000	0.926208000	-1.549444000	9	5.418042000	0.703621000	-1.682518000
9	-2.269308000	-2.772788000	-1.047880000	9	-2.335297000	-2.827592000	-0.857161000
9	-4.670125000	-1.533024000	-0.376094000	9	-4.726640000	-1.470597000	-0.259768000
9	-5.363054000	0.769194000	-1.586111000	9	-5.435447000	0.710943000	-1.669716000
9	-2.226444000	3.111568000	1.031824000	9	-2.260046000	3.282286000	0.665524000
9	-1.542897000	0.803762000	2.262706000	9	-1.489406000	1.074620000	2.035063000
9	-0.012433000	-1.526126000	2.881612000	9	-0.002982000	-1.172793000	2.870373000
9	2.399303000	-2.775733000	-0.953474000	9	2.334864000	-2.826843000	-0.854474000
9	1.428987000	0.801180000	2.297896000	9	1.502407000	1.083293000	2.052920000
9	1.958809000	3.115817000	1.017206000	9	2.269089000	3.286241000	0.676095000
9	3.851253000	3.176584000	-0.940052000	9	4.190349000	3.084298000	-1.236652000
9	-4.140871000	3.096738000	-0.902371000	9	-4.199052000	3.088056000	-1.229848000
9	0.091547000	-3.288286000	-2.251330000	9	0.000874000	-3.447967000	-2.058293000
9	1.037764000	-0.183579000	-1.979210000	8	1.105295000	-0.017515000	-1.572894000
9	0.710985000	2.070443000	-1.691421000	7	0.009427000	0.511318000	-1.254060000
9	0.028068000	0.598265000	-0.068372000	8	-0.000822000	1.578003000	-0.587702000
5	0.165975000	0.799849000	-1.472253000	8	-1.075226000	-0.030835000	-1.587971000
9	-1.105767000	0.678875000	-2.051293000				
R_{II...}ClO⁻				R_{II...}ClO₂⁻			
6	3.539167000	-2.067882000	-0.523564000	6	-4.462392000	1.841120000	-0.265397000
6	2.608163000	-2.062054000	0.502978000	6	-3.356381000	2.011459000	0.552007000
6	4.192399000	-0.896420000	-0.871737000	6	-4.972607000	0.570487000	-0.479186000
6	2.314041000	-0.870593000	1.147187000	6	-2.769782000	0.904560000	1.141261000
6	3.893606000	0.278554000	-0.195481000	6	-4.360493000	-0.520026000	0.118806000
6	2.946986000	0.326786000	0.818325000	6	-3.241049000	-0.386283000	0.929839000
6	-3.535498000	-2.071306000	-0.525110000	6	4.374681000	1.907993000	-0.427031000
6	-4.191604000	-0.900957000	-0.871680000	6	5.033673000	0.692566000	-0.320952000
6	-2.603943000	-2.064532000	0.500934000	6	3.140226000	2.082747000	0.178075000
6	-3.895162000	0.273912000	-0.194238000	6	4.445926000	-0.339376000	0.392475000
6	-2.311985000	-0.873122000	1.146188000	6	2.579286000	1.034200000	0.889415000
6	-2.947951000	0.323096000	0.819010000	6	3.211458000	-0.197643000	1.012549000
6	-0.003397000	3.088208000	-0.943490000	6	0.160287000	-2.576853000	-0.971783000
6	1.185171000	2.743028000	-0.328511000	6	-1.066411000	-2.345784000	-0.374520000
6	-1.191097000	2.741682000	-0.327646000	6	1.312197000	-2.259813000	-0.270587000
6	1.226852000	2.117119000	0.909529000	6	-1.183666000	-1.839284000	0.913433000
6	-1.231042000	2.115759000	0.910457000	6	1.269845000	-1.757538000	1.022745000
6	-0.001761000	1.869091000	1.511772000	6	0.008734000	-1.576226000	1.575384000
6	2.531582000	1.619589000	1.478376000	6	-2.534241000	-1.576543000	1.525163000
1	3.315823000	2.364420000	1.329372000	1	-3.171798000	-2.454681000	1.398272000
1	2.418425000	1.463381000	2.553117000	1	-2.403165000	-1.420882000	2.598588000
6	-2.534665000	1.616151000	1.479882000	6	2.533652000	-1.338983000	1.723111000
1	-2.420735000	1.459488000	2.554469000	1	2.284213000	-1.044040000	2.744797000
1	-3.320236000	2.359723000	1.331639000	1	3.231996000	-2.176874000	1.788661000
9	-4.580822000	1.380546000	-0.536378000	9	5.111301000	-1.506147000	0.475757000
9	-5.119776000	-0.915142000	-1.839636000	9	6.230425000	0.530722000	-0.902351000
9	2.332685000	3.026325000	-0.963924000	9	-2.176304000	-2.637518000	-1.065917000
9	4.576535000	1.386330000	-0.539400000	9	-4.890345000	-1.736321000	-0.106120000
9	5.120131000	-0.909537000	-1.840154000	9	-6.055926000	0.408325000	-1.252099000
9	2.023512000	-3.199402000	0.875792000	9	-2.871869000	3.235238000	0.764959000
9	1.485827000	-0.906301000	2.189979000	9	-1.716036000	1.093073000	1.935599000
9	-0.001203000	1.350363000	2.756019000	9	-0.060285000	-1.104668000	2.843888000
9	-2.339525000	3.023408000	-0.962167000	9	2.501209000	-2.490252000	-0.843130000

9	-1.483059000	-0.907949000	2.188398000	9	1.397896000	1.216480000	1.473668000
9	-2.017290000	-3.201203000	0.872611000	9	2.506636000	3.247939000	0.066504000
9	-3.824975000	-3.209306000	-1.161133000	9	4.930687000	2.906909000	-1.120232000
9	3.830745000	-3.205873000	-1.158656000	9	-5.038750000	2.899334000	-0.845276000
9	-0.004121000	3.708291000	-2.130999000	9	0.233450000	-3.093963000	-2.204240000
17	0.003849000	-1.547981000	-1.40712100	8	1.350067000	0.405416000	-1.395677000
8	0.001767000	-0.244118000	-0.282475000	17	-0.106507000	0.390061000	-2.07339800
				8	-1.323451000	0.564384000	-1.036882000
R_{II...}ClO₃⁻				R_{II...}ClO₄⁻			
6	-3.800506000	1.994813000	-0.452713000	6	3.820938000	-1.978397000	-0.237392000
6	-2.821593000	2.083909000	0.524169000	6	2.835851000	-1.998843000	0.738156000
6	-4.430579000	0.783838000	-0.694754000	6	4.438789000	-0.783053000	-0.572320000
6	-2.464012000	0.946049000	1.229984000	6	2.464491000	-0.810823000	1.347994000
6	-4.054806000	-0.336263000	0.028018000	6	4.051533000	0.387241000	0.059676000
6	-3.052292000	-0.291226000	0.990069000	6	3.048982000	0.408651000	1.022087000
6	3.800685000	1.994709000	-0.452657000	6	-3.826856000	-1.975518000	-0.238764000
6	4.430631000	0.783687000	-0.694798000	6	-4.445389000	-0.778706000	-0.567353000
6	2.821822000	2.083840000	0.524270000	6	-2.836468000	-1.999619000	0.731236000
6	4.054768000	-0.336425000	0.027910000	6	-4.053252000	0.389500000	0.065236000
6	2.464145000	0.945967000	1.230015000	6	-2.459989000	-0.813418000	1.341978000
6	3.052289000	-0.291352000	0.989998000	6	-3.045422000	0.407255000	1.022335000
6	-0.000116000	-2.864557000	-0.806716000	6	0.000296000	2.938966000	-0.905948000
6	-1.188095000	-2.551060000	-0.173849000	6	1.189823000	2.645522000	-0.264927000
6	1.187906000	-2.551125000	-0.173894000	6	-1.187879000	2.644294000	-0.263053000
6	-1.228449000	-1.971337000	1.088552000	6	1.231866000	2.107566000	1.015637000
6	1.228343000	-1.971406000	1.088503000	6	-1.227265000	2.106029000	1.017372000
6	-0.000036000	-1.721351000	1.689477000	6	0.002876000	1.881824000	1.627258000
6	-2.541338000	-1.529921000	1.683887000	6	2.543908000	1.692836000	1.632082000
1	-3.284983000	-2.324106000	1.588786000	1	3.292393000	2.474043000	1.484264000
1	-2.401706000	-1.327704000	2.747432000	1	2.408349000	1.561629000	2.707424000
6	2.541273000	-1.530038000	1.683790000	6	-2.537968000	1.689081000	1.635305000
1	2.401678000	-1.327831000	2.747342000	1	-2.399528000	1.553746000	2.709765000
1	3.284875000	-2.324259000	1.588659000	1	-3.286623000	2.471125000	1.492659000
9	4.710727000	-1.483248000	-0.211710000	9	-4.696677000	1.522950000	-0.257454000
9	5.401151000	0.710968000	-1.613470000	9	-5.420670000	-0.763855000	-1.482098000
9	-2.335439000	-2.815888000	-0.806350000	9	2.335390000	2.884924000	-0.910494000
9	-4.710893000	-1.483037000	-0.211498000	9	4.694233000	1.519142000	-0.269753000
9	-5.401137000	0.711154000	-1.613389000	9	5.408891000	-0.771260000	-1.492499000
9	-2.244756000	3.257145000	0.778451000	9	2.273239000	-3.151174000	1.088628000
9	-1.542930000	1.054650000	2.186485000	9	1.523112000	-0.848605000	2.292633000
9	0.000000000	-1.212478000	2.941770000	9	0.003833000	1.431715000	2.900003000
9	2.335211000	-2.816021000	-0.806443000	9	-2.334820000	2.882098000	-0.906652000
9	1.543100000	1.054606000	2.186545000	9	-1.513556000	-0.853876000	2.281398000
9	2.245096000	3.257110000	0.778641000	9	-2.272804000	-3.153564000	1.074640000
9	4.159046000	3.080756000	-1.143820000	9	-4.208351000	-3.105379000	-0.835328000
9	-4.158782000	3.080850000	-1.143933000	9	4.197879000	-3.110193000	-0.833115000
9	-0.000154000	-3.408680000	-2.023491000	9	-0.000900000	3.450763000	-2.137041000
17	-0.000056000	0.701814000	-1.62230600	17	0.000831000	-0.788358000	-1.52294100
8	-1.244010000	-0.154476000	-1.848599000	8	-0.003991000	-1.380301000	-0.158211000
8	0.000153000	1.116352000	-0.146088000	8	1.217039000	0.052914000	-1.674023000
8	1.243696000	-0.154680000	-1.848898000	8	-0.000347000	-1.859844000	-2.534345000
				8	-1.210339000	0.059237000	-1.678359000

$R_{II...SO_4^{2-}}$			
6	3.535730000	-2.044922000	-0.466964000
6	2.663702000	-2.081639000	0.605484000
6	4.169024000	-0.858363000	-0.803355000
6	2.399158000	-0.916172000	1.308856000
6	3.877336000	0.290476000	-0.093956000
6	2.972192000	0.303044000	0.960025000
6	-3.502022000	-2.062940000	-0.471291000
6	-4.150354000	-0.883732000	-0.805810000
6	-2.639046000	-2.092926000	0.608561000
6	-3.879394000	0.265895000	-0.089739000
6	-2.394221000	-0.926622000	1.317363000
6	-2.979145000	0.286896000	0.968567000
6	-0.013942000	3.112421000	-0.757081000
6	1.176520000	2.751684000	-0.157277000
6	-1.201551000	2.744074000	-0.155675000
6	1.221959000	2.089277000	1.063024000
6	-1.241731000	2.084619000	1.066352000
6	-0.008563000	1.791576000	1.637562000
6	2.527538000	1.583841000	1.626622000
1	3.305313000	2.340599000	1.495552000
1	2.406646000	1.411549000	2.698826000
6	-2.544007000	1.572469000	1.632457000
1	-2.421793000	1.404536000	2.705228000
1	-3.326815000	2.323609000	1.499173000
9	-4.539156000	1.390973000	-0.439871000
9	-5.041224000	-0.872640000	-1.816614000
9	2.321672000	3.097516000	-0.764435000
9	4.526361000	1.422033000	-0.442944000
9	5.067551000	-0.839863000	-1.807274000
9	2.105963000	-3.238351000	0.969965000
9	1.665441000	-1.003012000	2.423023000
9	-0.005485000	1.199372000	2.853166000
9	-2.349151000	3.083207000	-0.761144000
9	-1.660863000	-1.006814000	2.432467000
9	-2.068856000	-3.243410000	0.972753000
9	-3.760841000	-3.182349000	-1.161274000
9	3.818637000	-3.164990000	-1.147580000
9	-0.016856000	3.762778000	-1.931834000
16	-0.009376000	-0.549523000	-1.20549000
8	0.001196000	-0.789416000	0.307426000
8	1.239955000	0.220331000	-1.556225000
8	-0.044932000	-1.870220000	-1.902895000
8	-1.235867000	0.266591000	-1.533173000

Table S3. Cartesian coordinates (in Å) of **R_{III}...X** complexes.

R_{III}...N₂				R_{III}...O₃			
6	1.378761000	3.878464000	1.157846000	6	4.200107000	-1.250863000	1.910924000
6	0.100293000	3.341309000	1.082864000	6	4.792169000	-1.281290000	0.656142000
6	2.203803000	3.849963000	0.041668000	6	2.912210000	-1.741546000	2.072264000
6	-0.330846000	2.781569000	-0.109586000	6	4.089436000	-1.798162000	-0.430449000
6	1.742530000	3.280235000	-1.138496000	6	2.238941000	-2.254375000	0.966611000
6	0.470762000	2.727095000	-1.245521000	6	2.801512000	-2.296944000	-0.307155000
6	4.041760000	-1.733262000	1.864137000	6	-4.662417000	0.003426000	1.766721000
6	4.656125000	-1.420983000	0.659009000	6	-3.594958000	-0.868033000	1.937533000
6	2.785361000	-2.325069000	1.864434000	6	-5.228696000	0.164816000	0.509518000
6	4.003726000	-1.698335000	-0.535667000	6	-3.099248000	-1.551463000	0.838309000
6	2.161574000	-2.591288000	0.655410000	6	-4.713962000	-0.540271000	-0.570151000
6	2.741883000	-2.281516000	-0.570303000	6	-3.636574000	-1.409406000	-0.437728000
6	-4.585726000	-0.116060000	1.837539000	6	1.177710000	3.914605000	0.778717000
6	-3.550821000	-1.040816000	1.898546000	6	-0.095994000	3.372918000	0.663359000
6	-5.159692000	0.199083000	0.613435000	6	2.088748000	3.755678000	-0.255957000
6	-3.101800000	-1.631520000	0.727531000	6	-0.433874000	2.675344000	-0.485978000
6	-4.683668000	-0.405587000	-0.542397000	6	1.717362000	3.054169000	-1.396279000
6	-3.642779000	-1.326924000	-0.518115000	6	0.453268000	2.493046000	-1.542891000
6	0.779913000	-1.663741000	-2.001071000	6	-1.631884000	-1.645881000	-1.884929000
6	0.880079000	-0.291365000	-2.194074000	6	-0.499420000	-2.415286000	-1.646964000
6	-0.516902000	-2.162570000	-1.908457000	6	-1.397445000	-0.337900000	-2.294156000
6	-0.199322000	0.574633000	-2.328997000	6	0.804448000	-1.946475000	-1.780102000
6	-1.660719000	-1.377944000	-2.002258000	6	-0.138038000	0.233175000	-2.427720000
6	-1.448934000	-0.022685000	-2.234062000	6	0.928118000	-0.616397000	-2.160206000
6	2.002522000	-2.532996000	-1.859061000	6	-3.030880000	-2.131346000	-1.615614000
1	1.697352000	-3.580261000	-1.906974000	1	-3.664546000	-1.970450000	-2.490017000
1	2.684291000	-2.355472000	-2.693216000	1	-3.007061000	-3.205818000	-1.422438000
6	-0.013450000	2.058284000	-2.506909000	6	2.011819000	-2.797537000	-1.487561000
1	0.706072000	2.251807000	-3.304425000	1	1.684471000	-3.823125000	-1.302760000
1	-0.964451000	2.499523000	-2.812571000	1	2.669963000	-2.822159000	-2.358534000
6	-3.050709000	-1.912234000	-1.775271000	6	0.067050000	1.687041000	-2.758766000
1	-3.696659000	-1.666041000	-2.620382000	1	0.849468000	1.791308000	-3.511983000
1	-3.009332000	-3.000334000	-1.700394000	1	-0.854677000	2.087276000	-3.186570000
9	2.181164000	-2.607875000	3.015039000	9	-6.259324000	0.990940000	0.348358000
9	0.940103000	-3.135904000	0.678520000	9	-5.291549000	-0.368249000	-1.764090000
9	-2.106051000	-2.521336000	0.804008000	9	-1.659488000	2.136818000	-0.556470000
9	-3.002730000	-1.350144000	3.069476000	9	-0.972020000	3.514483000	1.651857000
9	4.631123000	-1.393664000	-1.675523000	9	-2.061230000	-2.378153000	1.019941000
9	5.863451000	-0.863820000	0.656367000	9	-3.063457000	-1.039868000	3.142224000
9	2.114930000	0.242442000	-2.256622000	9	-0.672300000	-3.691925000	-1.262487000
9	2.561163000	3.281249000	-2.194224000	9	0.994707000	-2.701064000	1.143381000
9	3.425156000	4.370452000	0.108558000	9	2.327939000	-1.712773000	3.260654000
9	-0.689021000	3.343752000	2.153428000	9	6.024036000	-0.815297000	0.498347000
9	-1.557393000	2.243214000	-0.146101000	9	4.696733000	-1.797252000	-1.618601000
9	-2.540514000	0.751195000	-2.370705000	9	2.171966000	-0.113573000	-2.270208000
9	-0.672968000	-3.484045000	-1.724022000	9	-2.473289000	0.419448000	-2.569292000
9	-5.255550000	-0.074713000	-1.704635000	9	2.618016000	2.934996000	-2.376261000
9	-6.155852000	1.079172000	0.555997000	9	3.307488000	4.277715000	-0.150998000
9	4.653041000	-1.466990000	3.012052000	9	-5.146526000	0.674065000	2.805339000
9	1.810578000	4.414873000	2.292390000	9	1.521582000	4.581132000	1.872941000
9	-5.031374000	0.458240000	2.948596000	9	4.862923000	-0.756436000	2.947009000

7	-0.215081000	-0.213403000	1.326248000	8	1.255761000	0.195304000	0.747394000
7	0.791806000	0.119327000	1.022542000	8	-0.004031000	-0.005688000	0.802545000
				8	-0.593044000	0.275591000	1.884132000
R_{III...}H₂O				R_{III...}H₂O₂			
6	4.338155000	-0.737974000	1.896909000	6	4.308787000	-0.673428000	1.933451000
6	4.878513000	-0.876181000	0.625325000	6	4.897413000	-0.825231000	0.684596000
6	3.108119000	-1.311793000	2.187744000	6	3.087128000	-1.277868000	2.194299000
6	4.175587000	-1.576956000	-0.345741000	6	4.246140000	-1.562853000	-0.295341000
6	2.438529000	-2.012970000	1.199095000	6	2.476412000	-2.027251000	1.203822000
6	2.937650000	-2.156204000	-0.089036000	6	3.017922000	-2.173832000	-0.066567000
6	-4.455439000	0.385608000	1.725326000	6	-4.515770000	0.272374000	1.663321000
6	-3.331772000	-0.370072000	2.033047000	6	-3.374922000	-0.442775000	2.004635000
6	-5.127965000	0.160486000	0.531901000	6	-5.137251000	0.041585000	0.443672000
6	-2.901416000	-1.334751000	1.137403000	6	-2.867624000	-1.364801000	1.103024000
6	-4.662865000	-0.808708000	-0.347752000	6	-4.610987000	-0.902463000	-0.427901000
6	-3.536765000	-1.577070000	-0.075182000	6	-3.464086000	-1.627853000	-0.125787000
6	0.932577000	3.816126000	0.446942000	6	0.765285000	3.926673000	0.349042000
6	-0.298174000	3.175848000	0.439262000	6	-0.450613000	3.259102000	0.304087000
6	1.791425000	3.668945000	-0.633932000	6	1.695831000	3.735743000	-0.662795000
6	-0.651187000	2.392653000	-0.646327000	6	-0.708589000	2.395350000	-0.747555000
6	1.411034000	2.872696000	-1.706075000	6	1.398270000	2.878116000	-1.713381000
6	0.187675000	2.211443000	-1.740707000	6	0.194221000	2.186189000	-1.786100000
6	-1.594464000	-2.029099000	-1.525134000	6	-1.484440000	-2.079049000	-1.539732000
6	-0.400317000	-2.678345000	-1.235158000	6	-0.287797000	-2.719664000	-1.238079000
6	-1.474679000	-0.782358000	-2.129470000	6	-1.368776000	-0.843220000	-2.168210000
6	0.859304000	-2.144727000	-1.492589000	6	0.970977000	-2.184415000	-1.504837000
6	-0.270290000	-0.143140000	-2.382604000	6	-0.167421000	-0.198172000	-2.421430000
6	0.864814000	-0.869323000	-2.044145000	6	0.971414000	-0.914571000	-2.073500000
6	-2.942728000	-2.533160000	-1.080431000	6	-2.833136000	-2.587405000	-1.104786000
1	-3.624103000	-2.624989000	-1.928479000	1	-3.497432000	-2.703387000	-1.963552000
1	-2.832085000	-3.526794000	-0.642054000	1	-2.717950000	-3.572232000	-0.647812000
6	2.139418000	-2.863291000	-1.152965000	6	2.254123000	-2.891772000	-1.148498000
1	1.897232000	-3.874485000	-0.819460000	1	2.018337000	-3.907574000	-0.824775000
1	2.759270000	-2.959949000	-2.047102000	1	2.890818000	-2.974391000	-2.031900000
6	-0.189841000	1.280039000	-2.866228000	6	-0.102023000	1.223121000	-2.910633000
1	0.549858000	1.370356000	-3.663240000	1	0.671948000	1.325045000	-3.672625000
1	-1.156462000	1.572235000	-3.281755000	1	-1.055212000	1.483801000	-3.375590000
9	-6.206418000	0.879348000	0.234890000	9	-6.232642000	0.722715000	0.120589000
9	-5.325812000	-0.982162000	-1.494648000	9	-5.237390000	-1.099038000	-1.592319000
9	-1.836109000	1.772060000	-0.613423000	9	-1.870008000	1.727098000	-0.736450000
9	-1.114129000	3.283909000	1.488219000	9	-1.347620000	3.446880000	1.266058000
9	-1.805010000	-2.048543000	1.455593000	9	-1.743876000	-2.030547000	1.434102000
9	-2.676656000	-0.163003000	3.174288000	9	-2.800714000	-0.250669000	3.186866000
9	-0.468557000	-3.893457000	-0.659529000	9	-0.350881000	-3.925125000	-0.643866000
9	1.249541000	-2.559545000	1.501786000	9	1.293007000	-2.598955000	1.477842000
9	2.576244000	-1.174666000	3.401209000	9	2.491370000	-1.107298000	3.375550000
9	6.060570000	-0.334370000	0.346435000	9	6.072322000	-0.255924000	0.434178000
9	4.723960000	-1.685159000	-1.559980000	9	4.832823000	-1.672846000	-1.490738000
9	2.060118000	-0.290081000	-2.263757000	9	2.163785000	-0.329920000	-2.286652000
9	-2.617226000	-0.150636000	-2.456647000	9	-2.512154000	-0.231551000	-2.521279000
9	2.261989000	2.756900000	-2.731332000	9	2.311330000	2.735233000	-2.681848000
9	2.967737000	4.291319000	-0.634966000	9	2.858182000	4.384125000	-0.626247000
9	-4.888276000	1.312431000	2.570535000	9	-5.020345000	1.161552000	2.509239000
9	1.288815000	4.565472000	1.485365000	9	1.037071000	4.750135000	1.356503000

9	4.996046000	-0.061098000	2.831207000	9	4.910354000	0.048449000	2.871372000
8	0.216613000	0.189025000	1.227831000	8	0.418765000	0.033511000	0.764332000
1	-0.098305000	-0.701511000	1.416914000	1	-0.054366000	-0.810463000	0.670552000
1	0.200862000	0.618153000	2.088433000	8	-0.364937000	0.676026000	1.796676000
				1	0.158798000	0.484310000	2.588621000
R_{III...}F⁻				R_{III...}Cl⁻			
6	-3.098581000	0.970957000	1.892207000	6	3.900173000	-0.035151000	1.852903000
6	-2.474070000	-0.225283000	1.584974000	6	3.161564000	1.086531000	1.514382000
6	-3.726246000	1.703594000	0.893000000	6	4.350486000	-0.892617000	0.859879000
6	-2.475910000	-0.672798000	0.272944000	6	2.865216000	1.323764000	0.181924000
6	-3.698927000	1.239577000	-0.410814000	6	4.046195000	-0.624080000	-0.465342000
6	-3.071341000	0.048150000	-0.758021000	6	3.286443000	0.478358000	-0.839401000
6	2.388694000	2.204200000	1.889963000	6	-2.045109000	-3.180680000	1.873587000
6	1.040613000	2.259332000	1.581237000	6	-0.694821000	-3.156219000	1.565761000
6	3.338036000	2.378202000	0.891237000	6	-2.987392000	-3.160172000	0.855662000
6	0.655276000	2.479721000	0.268050000	6	-0.305748000	-3.086440000	0.237589000
6	2.923812000	2.581741000	-0.413736000	6	-2.567910000	-3.103763000	-0.463962000
6	1.578647000	2.631865000	-0.762347000	6	-1.221797000	-3.049718000	-0.808786000
6	0.712865000	-3.161069000	1.897814000	6	-1.916115000	3.306161000	1.827301000
6	1.436116000	-2.023258000	1.584394000	6	-2.486799000	2.090101000	1.489893000
6	0.390529000	-4.075282000	0.903140000	6	-1.428339000	4.141165000	0.832798000
6	1.819424000	-1.805207000	0.270286000	6	-2.544368000	1.717066000	0.156745000
6	0.775495000	-3.824452000	-0.402657000	6	-1.509558000	3.745601000	-0.492949000
6	1.490546000	-2.685601000	-0.756332000	6	-2.057757000	2.524067000	-0.866837000
6	0.535100000	1.308730000	-2.535733000	6	-0.342049000	-1.406391000	-2.438393000
6	-0.827192000	1.065767000	-2.546651000	6	0.979692000	-0.991134000	-2.431297000
6	1.339956000	0.174444000	-2.546527000	6	-1.285729000	-0.385751000	-2.473569000
6	-1.407306000	-0.198388000	-2.534265000	6	1.391222000	0.337884000	-2.441187000
6	0.869004000	-1.126762000	-2.534820000	6	-0.985331000	0.966082000	-2.469530000
6	-0.515815000	-1.256748000	-2.545641000	6	0.370844000	1.275100000	-2.463065000
6	1.117170000	2.658540000	-2.202039000	6	-0.756906000	-2.840540000	-2.230860000
1	1.963776000	2.897643000	-2.848273000	1	-1.566274000	-3.105601000	-2.914230000
1	0.357141000	3.429053000	-2.345961000	1	0.089901000	-3.495672000	-2.443971000
6	-2.866769000	-0.368457000	-2.197111000	6	2.841172000	0.709039000	-2.264020000
1	-3.498606000	0.243291000	-2.843719000	1	3.468342000	0.115833000	-2.932730000
1	-3.154293000	-1.412342000	-2.337300000	1	2.975400000	1.760491000	-2.525789000
6	1.745954000	-2.305264000	-2.197361000	6	-2.034909000	2.032456000	-2.294968000
1	1.528861000	-3.159601000	-2.841050000	1	-1.836488000	2.876302000	-2.958554000
1	2.793483000	-2.033424000	-2.341868000	1	-3.011403000	1.621588000	-2.559515000
9	4.644112000	2.351638000	1.199907000	9	-4.291340000	-3.227133000	1.153407000
9	3.871941000	2.744180000	-1.357639000	9	-3.511605000	-3.138479000	-1.421164000
9	2.591017000	-0.751966000	-0.002578000	9	-3.108930000	0.546631000	-0.147796000
9	1.755062000	-1.153446000	2.539860000	9	-2.967272000	1.294481000	2.440757000
9	-0.643448000	2.621974000	-0.000139000	9	0.999579000	-3.079760000	-0.040311000
9	0.131570000	2.102009000	2.540518000	9	0.209063000	-3.197275000	2.539811000
9	-1.668439000	2.123302000	-2.515322000	9	1.946391000	-1.931181000	-2.409263000
9	-4.317142000	1.976257000	-1.354846000	9	4.538214000	-1.455620000	-1.400590000
9	-4.356345000	2.848295000	1.200449000	9	5.098153000	-1.954888000	1.186114000
9	-1.880013000	-0.931202000	2.544078000	9	2.743961000	1.918537000	2.463892000
9	-1.950134000	-1.869660000	0.007197000	9	2.172369000	2.421537000	-0.125856000
9	-1.010957000	-2.514158000	-2.512612000	9	0.699045000	2.583423000	-2.475256000
9	2.676422000	0.374631000	-2.515013000	9	-2.583093000	-0.753598000	-2.505433000
9	0.446001000	-4.732805000	-1.342055000	9	-1.061017000	4.600153000	-1.429567000

9	-0.284622000	-5.192386000	1.216424000	9	-0.908785000	5.331811000	1.158367000
9	2.784526000	1.996352000	3.149350000	9	-2.443730000	-3.242506000	3.145613000
9	0.334203000	-3.394098000	3.158143000	9	-1.844025000	3.683659000	3.105206000
9	-3.114610000	1.420497000	3.150733000	9	4.194195000	-0.286218000	3.130257000
9	-0.004793000	0.000350000	0.232102000	17	0.047985000	0.016504000	0.835033000
R_{III...}BF₄⁻				R_{III...}NO₃⁻			
6	4.052378000	-1.571595000	1.712739000	6	-1.412123000	3.664268000	1.504006000
6	4.566208000	-0.993043000	0.562032000	6	-2.406221000	3.437670000	0.564757000
6	2.940740000	-2.396599000	1.638113000	6	-0.079929000	3.569149000	1.135848000
6	3.960665000	-1.244137000	-0.658931000	6	-2.053668000	3.086803000	-0.727957000
6	2.336360000	-2.601305000	0.407188000	6	0.243740000	3.220816000	-0.165231000
6	2.829254000	-2.044274000	-0.768605000	6	-0.727834000	2.940782000	-1.119551000
6	-4.021066000	-0.531779000	1.922475000	6	4.026966000	-0.460844000	1.951894000
6	-3.038306000	-1.506379000	1.823358000	6	4.506947000	0.366682000	0.948117000
6	-4.711054000	-0.126532000	0.789150000	6	3.302192000	-1.596077000	1.627410000
6	-2.746290000	-2.045930000	0.580242000	6	4.240825000	0.060334000	-0.376222000
6	-4.398035000	-0.686550000	-0.440266000	6	3.041363000	-1.869873000	0.294751000
6	-3.399230000	-1.642880000	-0.581303000	6	3.487672000	-1.051249000	-0.737794000
6	0.707078000	4.062993000	1.044430000	6	-3.370097000	-2.090538000	1.865472000
6	-0.556237000	3.523652000	0.858003000	6	-2.213197000	-2.800339000	1.588379000
6	1.653608000	3.973389000	0.036054000	6	-4.100621000	-1.523062000	0.831848000
6	-0.841937000	2.872780000	-0.331897000	6	-1.787004000	-2.908454000	0.274539000
6	1.327802000	3.343582000	-1.154203000	6	-3.654219000	-1.654853000	-0.472663000
6	0.078920000	2.773534000	-1.370308000	6	-2.479107000	-2.330292000	-0.783861000
6	-1.598266000	-1.498921000	-2.251700000	6	1.629477000	-0.888739000	-2.363342000
6	-0.389416000	-2.178116000	-2.173202000	6	1.286656000	0.457975000	-2.435721000
6	-1.506507000	-0.128608000	-2.464543000	6	0.565396000	-1.783837000	-2.347185000
6	0.854433000	-1.561906000	-2.247855000	6	-0.012801000	0.943404000	-2.455033000
6	-0.319747000	0.581741000	-2.540009000	6	-0.771074000	-1.399567000	-2.335926000
6	0.830794000	-0.183722000	-2.409864000	6	-0.999733000	-0.030040000	-2.380840000
6	-2.927592000	-2.133166000	-1.929809000	6	3.062715000	-1.312958000	-2.163444000
1	-3.673558000	-1.878736000	-2.685599000	1	3.160334000	-2.376064000	-2.391051000
1	-2.818865000	-3.219069000	-1.918998000	1	3.719283000	-0.762254000	-2.839836000
6	2.153270000	-2.306699000	-2.090955000	6	-0.344630000	2.415585000	-2.480080000
1	1.958253000	-3.376768000	-2.188759000	1	0.522098000	2.965298000	-2.852188000
1	2.839368000	-2.023111000	-2.892578000	1	-1.171693000	2.589114000	-3.172248000
6	-0.269142000	2.080454000	-2.664529000	6	-1.913656000	-2.371425000	-2.182195000
1	0.471132000	2.361888000	-3.416611000	1	-2.706895000	-2.129580000	-2.892945000
1	1.241999000	2.435679000	-3.011613000	1	-1.558735000	-3.378772000	-2.408150000
9	-5.685621000	0.784151000	0.892627000	9	2.883088000	-2.412018000	2.589655000
9	-5.109425000	-0.288843000	-1.508922000	9	2.347817000	-2.970997000	-0.004870000
9	-2.062258000	2.347270000	-0.487502000	9	-0.681547000	-3.610797000	0.018235000
9	-1.479906000	3.657154000	1.802935000	9	-1.536969000	-3.377832000	2.576738000
9	-1.800343000	-2.980985000	0.497668000	9	4.762335000	0.860821000	-1.321195000
9	-2.395935000	-1.912481000	2.910199000	9	5.241610000	1.439075000	1.265344000
9	-0.426182000	-3.518460000	-2.017279000	9	2.298771000	1.342074000	-2.496244000
9	1.260619000	-3.389175000	0.348513000	9	1.532656000	3.187575000	-0.508590000
9	2.486783000	-2.994668000	2.732596000	9	0.876029000	3.815101000	2.032851000
9	5.655221000	-0.220428000	0.635620000	9	-3.691980000	3.573025000	0.909953000
9	4.521389000	-0.712512000	-1.757421000	9	-3.043960000	2.907405000	-1.616538000
9	2.012674000	0.457706000	-2.459341000	9	-2.279718000	0.379778000	-2.370354000
9	-2.667620000	0.549457000	-2.582646000	9	0.845281000	-3.103173000	-2.363988000
9	2.256280000	3.320550000	-2.124593000	9	-4.410861000	-1.128787000	-1.449778000

9	2.865156000	4.511718000	0.210814000	9	-5.237768000	-0.871033000	1.100653000
9	-4.325936000	-0.006303000	3.107310000	9	4.288750000	-0.175581000	3.229305000
9	1.007791000	4.685895000	2.184667000	9	-3.797938000	-1.972280000	3.124598000
9	4.645347000	-1.352287000	2.886876000	9	-1.739983000	4.002958000	2.753418000
5	0.254248000	0.106627000	1.403838000	7	0.118844000	-0.078669000	0.874045000
9	1.367048000	0.787116000	0.858668000	8	-1.055099000	0.311417000	0.639435000
9	0.687580000	-0.903261000	2.267276000	8	1.095520000	0.674801000	0.619261000
9	-0.582531000	1.005373000	2.081036000	8	0.321451000	-1.220319000	1.348245000
9	-0.476542000	-0.472867000	0.334250000				
R_{III...}ClO⁻				R_{III...}ClO₂⁻			
6	-1.048103000	3.700482000	0.876746000	6	0.758341000	3.725833000	1.023912000
6	-1.937709000	3.647672000	-0.183211000	6	-0.535648000	3.303189000	0.763164000
6	0.220771000	3.155845000	0.741997000	6	1.725378000	3.646104000	0.034810000
6	-1.545567000	3.056862000	-1.377349000	6	-0.839229000	2.778706000	-0.481860000
6	0.568738000	2.541480000	-0.449244000	6	1.392474000	3.119264000	-1.201407000
6	-0.291150000	2.489239000	-1.542830000	6	0.116089000	2.652889000	-1.485904000
6	3.953427000	0.067700000	1.964356000	6	4.122712000	-1.282818000	1.828869000
6	4.647227000	0.354290000	0.798667000	6	4.657912000	-0.894290000	0.611338000
6	3.011094000	-0.951597000	1.979050000	6	2.990324000	-2.082167000	1.861310000
6	4.385842000	-0.376654000	-0.350872000	6	4.045680000	-1.299483000	-0.563781000
6	2.749065000	-1.644719000	0.805919000	6	2.396444000	-2.464945000	0.670593000
6	3.426685000	-1.381427000	-0.383799000	6	2.896871000	-2.078975000	-0.567207000
6	-3.778384000	-1.269944000	1.918878000	6	-4.306429000	-0.286200000	1.907335000
6	-2.620024000	-2.033227000	1.944356000	6	-3.217281000	-1.140499000	1.953592000
6	-4.384395000	-0.972691000	0.709428000	6	-4.984381000	-0.093575000	0.711996000
6	-2.067624000	-2.461951000	0.748495000	6	-2.807879000	-1.782846000	0.796349000
6	-3.825069000	-1.445409000	-0.470137000	6	-4.551653000	-0.749336000	-0.430010000
6	-2.653486000	-2.188022000	-0.483425000	6	-3.456236000	-1.604150000	-0.420906000
6	1.687744000	-1.625909000	-2.100819000	6	0.888837000	-1.694397000	-2.021726000
6	1.502627000	-0.300966000	-2.475638000	6	0.879861000	-0.339401000	-2.331112000
6	0.528050000	-2.370237000	-1.928066000	6	-0.358792000	-2.283878000	-1.865368000
6	0.271297000	0.312862000	-2.618126000	6	-0.267060000	0.423104000	-2.516590000
6	-0.753568000	-1.855923000	-2.072604000	6	-1.561065000	-1.605833000	-2.009594000
6	-0.824614000	-0.510090000	-2.400358000	6	-1.460041000	-0.263270000	-2.351457000
6	3.046008000	-2.100184000	-1.657775000	6	2.179552000	-2.449086000	-1.838999000
1	3.017866000	-3.177917000	-1.485426000	1	1.962745000	-3.519663000	-1.835382000
1	3.803076000	-1.902178000	-2.419272000	1	2.845160000	-2.251600000	-2.682409000
6	0.115635000	1.794614000	-2.818840000	6	-0.203426000	1.910120000	-2.759151000
1	1.063470000	2.207079000	-3.173058000	1	0.562796000	2.133566000	-3.504231000
1	-0.637249000	1.997172000	-3.583087000	1	-1.163260000	2.247683000	-3.155834000
6	-1.998841000	-2.642927000	-1.763033000	6	-2.896606000	-2.217038000	-1.680159000
1	-2.718514000	-2.540847000	-2.578804000	1	-3.605098000	-2.059739000	-2.496325000
1	-1.738768000	-3.700731000	-1.684445000	1	-2.775719000	-3.294636000	-1.550926000
9	2.417445000	-1.281603000	3.120197000	9	2.481288000	-2.465584000	3.035251000
9	1.854476000	-2.629486000	0.835138000	9	1.295844000	-3.224295000	0.722952000
9	-0.962801000	-3.206996000	0.792236000	9	-1.764414000	-2.611488000	0.863425000
9	-2.075130000	-2.369113000	3.113111000	9	-2.558865000	-1.317441000	3.097529000
9	5.109053000	-0.093912000	-1.447637000	9	4.602038000	-0.916202000	-1.723091000
9	5.577541000	1.316667000	0.796524000	9	5.761441000	-0.140183000	0.580677000
9	2.617828000	0.440653000	-2.667247000	9	2.067357000	0.258955000	-2.515428000
9	1.798937000	2.029334000	-0.554077000	9	2.357291000	3.055338000	-2.132913000
9	1.095129000	3.251083000	1.743752000	9	2.969253000	4.070275000	0.283856000
9	-3.156609000	4.189658000	-0.060209000	9	-1.469469000	3.399635000	1.711454000
9	-2.427406000	3.060002000	-2.393665000	9	-2.101146000	2.418042000	-0.731597000

9	-2.048107000	0.040838000	-2.514740000	9	-2.620407000	0.402860000	-2.528836000
9	0.657246000	-3.671560000	-1.584358000	9	-0.408557000	-3.603929000	-1.574735000
9	-4.469185000	-1.172615000	-1.618913000	9	-5.237031000	-0.544431000	-1.568764000
9	-5.518735000	-0.260149000	0.688238000	9	-6.052909000	0.712980000	0.673459000
9	4.224774000	0.744112000	3.081101000	9	4.704794000	-0.900422000	2.968326000
9	-4.321431000	-0.839964000	3.060579000	9	-4.712519000	0.345777000	3.011087000
9	-1.408148000	4.284305000	2.021989000	9	1.071205000	4.223815000	2.224332000
17	-0.310015000	0.230755000	1.84756200	17	0.458203000	0.149093000	1.373700000
8	-0.314698000	-0.152715000	0.167096000	8	1.658149000	0.526310000	0.368130000
				8	-0.997063000	0.230486000	0.690761000
R_{III}...ClO₃⁻				R_{III}...ClO₄⁻			
6	3.696589000	-1.590108000	1.928960000	6	0.878217000	3.941286000	-1.167395000
6	4.364735000	-0.965595000	0.887283000	6	1.873373000	3.785242000	-0.216426000
6	2.662989000	-2.473278000	1.659541000	6	-0.430814000	3.604501000	-0.857090000
6	3.975028000	-1.216242000	-0.418213000	6	1.555920000	3.268780000	1.030312000
6	2.286893000	-2.697303000	0.344753000	6	-0.716547000	3.083091000	0.393256000
6	2.915886000	-2.063741000	-0.722130000	6	0.263580000	2.882474000	1.361281000
6	-3.933872000	-1.158777000	1.905750000	6	-4.291489000	-0.658947000	-1.849928000
6	-3.037093000	-2.175213000	1.619592000	6	-4.919271000	-0.158963000	-0.719161000
6	-4.485445000	-0.412455000	0.876233000	6	-3.270582000	-1.589404000	-1.721279000
6	-2.683288000	-2.417071000	0.301897000	6	-4.513601000	-0.588031000	0.535659000
6	-4.114644000	-0.676909000	-0.432335000	6	-2.879185000	-1.988598000	-0.453305000
6	-3.191513000	-1.666330000	-0.753153000	6	-3.479545000	-1.500425000	0.703604000
6	0.364443000	4.301616000	1.281773000	6	3.978448000	-1.760803000	-1.676987000
6	-0.860400000	4.073612000	0.676078000	6	2.870154000	-2.583366000	-1.549804000
6	1.529476000	3.917227000	0.638020000	6	4.515444000	-1.144757000	-0.556861000
6	-0.905054000	3.446944000	-0.558673000	6	2.297441000	-2.754510000	-0.299135000
6	1.452798000	3.290786000	-0.595634000	6	3.929563000	-1.346624000	0.682259000
6	0.240418000	3.020652000	-1.220760000	6	2.800532000	-2.141383000	0.843046000
6	-1.313582000	-1.252898000	-2.325533000	6	-1.586312000	-1.294339000	2.291595000
6	-0.136876000	-1.989460000	-2.304912000	6	-1.425433000	0.074232000	2.469058000
6	-1.161006000	0.126171000	-2.404169000	6	-0.414989000	-2.038602000	2.230224000
6	1.130894000	-1.422537000	-2.315632000	6	-0.201749000	0.721580000	2.548282000
6	0.056641000	0.790096000	-2.449225000	6	0.859662000	-1.488232000	2.295858000
6	1.170242000	-0.035755000	-2.391387000	6	0.907418000	-0.107372000	2.444140000
6	-2.677688000	-1.872170000	-2.157689000	6	-2.949689000	-1.890606000	2.061586000
1	-3.381045000	-1.426040000	-2.863904000	1	-2.880813000	-2.978003000	2.134387000
1	-2.616966000	-2.940363000	-2.375312000	1	-3.648949000	-1.549680000	2.827719000
6	2.392722000	-2.225376000	-2.127597000	6	-0.068337000	2.218281000	2.673548000
1	2.184574000	-3.278611000	-2.325366000	1	-1.005821000	2.625339000	3.057484000
1	3.159711000	-1.896373000	-2.832058000	1	0.716971000	2.454264000	3.394955000
6	0.166387000	2.292970000	-2.542749000	6	2.117751000	-2.309388000	2.176813000
1	1.060421000	2.539237000	-3.120463000	1	2.817838000	-2.023785000	2.965625000
1	-0.697213000	2.670679000	-3.094924000	1	1.863916000	-3.361158000	2.324974000
9	-5.379371000	0.542543000	1.153961000	9	-2.680179000	-2.077872000	-2.804813000
9	-4.698370000	0.043598000	-1.402234000	9	-1.891282000	-2.875710000	-0.341662000
9	-2.105596000	3.267297000	-1.115167000	9	1.232542000	-3.554213000	-0.192407000
9	-1.985262000	4.463751000	1.282658000	9	2.383909000	-3.211448000	-2.615965000
9	-1.848363000	-3.424260000	0.045788000	9	-5.176482000	-0.110979000	1.602284000
9	-2.530956000	-2.909687000	2.609975000	9	-5.923017000	0.715580000	-0.845232000
9	-0.228653000	-3.335344000	-2.296705000	9	-2.550147000	0.809516000	2.573554000
9	1.307142000	-3.567933000	0.100940000	9	-1.986797000	2.776559000	0.673427000
9	2.050381000	-3.099011000	2.663793000	9	-1.395696000	3.776491000	-1.757175000
9	5.384427000	-0.141261000	1.149714000	9	3.130204000	4.136865000	-0.504963000

9	4.674795000	-0.630436000	-1.402679000	9	2.544777000	3.160235000	1.931100000
9	2.384587000	0.539091000	-2.431498000	9	2.120846000	0.462904000	2.529009000
9	-2.286599000	0.858443000	-2.468024000	9	-0.524510000	-3.379862000	2.127940000
9	2.602778000	2.948844000	-1.184369000	9	4.505264000	-0.768536000	1.748010000
9	2.714834000	4.154697000	1.208419000	9	5.605972000	-0.380645000	-0.678479000
9	-4.286935000	-0.914531000	3.170644000	9	-4.684337000	-0.259494000	-3.059511000
9	0.422068000	4.907742000	2.471251000	9	4.546606000	-1.581525000	-2.870166000
9	4.066488000	-1.359088000	3.191515000	9	1.176436000	4.427691000	-2.370033000
8	-0.136968000	-1.394993000	0.925205000	17	0.246826000	0.179217000	-1.37618500
17	-0.033746000	0.095495000	1.23136700	8	0.230611000	1.163696000	-2.477581000
8	1.254161000	0.602871000	0.579241000	8	1.430250000	0.425396000	-0.505307000
8	-1.227999000	0.781469000	0.563858000	8	0.310291000	-1.194107000	-1.915877000
				8	-0.991894000	0.328217000	-0.557883000
R_{III...}SO₄²⁻							
6	3.591797000	-1.133834000	1.978028000				
6	4.260819000	-0.546476000	0.915238000				
6	2.639877000	-2.112489000	1.745231000				
6	3.958740000	-0.930014000	-0.377728000				
6	2.347613000	-2.463367000	0.437056000				
6	2.980672000	-1.878015000	-0.653996000				
6	-3.592888000	-1.136316000	1.977550000				
6	-2.639959000	-2.114035000	1.744975000				
6	-4.261932000	-0.549237000	0.914612000				
6	-2.346784000	-2.464399000	0.436860000				
6	-3.958855000	-0.932177000	-0.378279000				
6	-2.979811000	-1.879234000	-0.654299000				
6	-0.000826000	4.044592000	1.116905000				
6	-1.196150000	3.767144000	0.479324000				
6	1.195104000	3.763588000	0.481989000				
6	-1.181217000	3.172069000	-0.770443000				
6	1.181157000	3.168601000	-0.767814000				
6	0.000188000	2.845658000	-1.426076000				
6	-1.225081000	-1.507367000	-2.369451000				
6	0.000825000	-2.155331000	-2.310238000				
6	-1.166183000	-0.126874000	-2.535830000				
6	1.226764000	-1.507490000	-2.370091000				
6	0.000879000	0.612070000	-2.646267000				
6	1.167858000	-0.127091000	-2.537122000				
6	-2.532495000	-2.191168000	-2.063539000				
1	-3.307118000	-1.862981000	-2.761063000				
1	-2.410517000	-3.270533000	-2.181187000				
6	2.534228000	-2.190859000	-2.063361000				
1	2.412615000	-3.270324000	-2.180443000				
1	3.309121000	-1.862822000	-2.760654000				
6	0.000648000	2.118070000	-2.750715000				
1	0.883247000	2.428790000	-3.316328000				
1	-0.882142000	2.428302000	-3.316285000				
9	-5.223753000	0.359622000	1.152933000				
9	-4.667416000	-0.373072000	-1.382613000				
9	-2.362368000	2.944097000	-1.364437000				
9	-2.358624000	4.052762000	1.085570000				
9	-1.449470000	-3.432289000	0.222235000				
9	-2.084424000	-2.753155000	2.771903000				
9	0.000805000	-3.510005000	-2.209366000				

9	1.451138000	-3.432021000	0.222287000
9	2.084739000	-2.752219000	2.772013000
9	5.221947000	0.363060000	1.153789000
9	4.667439000	-0.370639000	-1.381798000
9	2.343802000	0.520216000	-2.640927000
9	-2.341972000	0.520840000	-2.638484000
9	2.362798000	2.937802000	-1.359614000
9	2.356968000	4.045542000	1.090890000
9	-3.911003000	-0.791209000	3.232645000
9	-0.001373000	4.599634000	2.332823000
9	3.909218000	-0.788333000	3.233171000
8	1.237671000	0.459900000	0.123159000
16	-0.000441000	0.274337000	0.98163400
8	-0.000928000	-1.137191000	1.519473000
8	-1.238338000	0.460471000	0.122993000
8	-0.000171000	1.276617000	2.091566000

Table S4. Binding energy values of receptor-guest complexes in aqueous phase using PCM solvation model in kcal/mol.

X	E _{int-PCM} (kcal/mol)		
	R _{I...X}	R _{II...X}	R _{III...X}
H ₂ O ₂	-3.20	-3.66	-4.91
H ₂ O	-1.52	-2.31	-4.08
O ₃	-5.48	-5.28	-7.83
N ₂	-2.21	-2.99	-4.58
Cl ₂	-4.63	-5.72	-6.91
Cl ⁻	-0.80	-0.16	0.54
F ⁻	4.32	9.36	6.56
BF ₄ ⁻	-2.85	-1.91	-2.29
NO ₃ ⁻	-3.27	-3.07	-2.28
SO ₄ ²⁻	5.05	8.02	8.47
ClO ⁻	-0.61	1.56	-1.28
ClO ₂ ⁻	-3.07	-2.99	-2.01
ClO ₃ ⁻	-3.48	-4.58	-4.56
ClO ₄ ⁻	-4.48	-4.00	-4.81

Table S5. Electron density (ρ) and Laplacian of electron density ($\nabla^2\rho$) in au for $R_I...X$, $R_{II}...X$ and $R_{III}...X$ complexes at their lone pair- π BCPs.

X	$R_I...X$		$R_{II}...X$		$R_{III}...X$	
	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$
H ₂ O ₂	0.006	0.024	0.006	0.025	0.010	0.036
	0.008	0.029	0.006	0.023	0.009	0.031
H ₂ O	0.009	0.031	0.002	0.010	0.003	0.011
	0.008	0.027	0.002	0.001	0.009	0.032
			0.009	0.033		
O ₃	0.012	0.042	0.013	0.048	0.009	0.030
	0.006	0.021	0.010	0.038	0.009	0.030
			0.008	0.035	0.007	0.029
					0.006	0.022
N ₂	0.006	0.021	0.006	0.023	0.005	0.017
	0.006	0.022	0.006	0.020	0.007	0.026
			0.006	0.027	0.004	0.018
					0.007	0.022
Cl ₂	0.012	0.045	0.006	0.020	0.006	0.020
	0.005	0.017	0.007	0.022	0.014	0.048
			0.010	0.036	0.008	0.029
Cl ⁻	0.011	0.035	0.010	0.031	0.007	0.021
	0.011	0.035	0.007	0.022	0.011	0.035
			0.010	0.031	0.011	0.036
					0.011	0.037
F ⁻	0.018	0.063	0.023	0.078	0.009	0.032
	0.016	0.055	0.015	0.052	0.019	0.067
			0.023	0.079	0.019	0.067
					0.019	0.068
BF ₄ ⁻	0.011	0.045	0.009	0.038	0.009	0.038
	0.012	0.047	0.007	0.028	0.010	0.043
			0.004	0.015	0.004	0.019
					0.005	0.022
NO ₃ ⁻	0.013	0.043	0.011	0.039	0.010	0.035
	0.008	0.029	0.009	0.032	0.010	0.035
			0.008	0.026	0.010	0.036
					0.010	0.035
SO ₄ ²⁻	0.019	0.061	0.013	0.043	0.017	0.057
	0.019	0.062	0.010	0.036	0.017	0.065
			0.019	0.066	0.014	0.049
					0.015	0.055
ClO ⁻	0.028	0.091	0.015	0.044	0.015	0.067
	0.016	0.051	0.012	0.054	0.012	0.038
			0.015	0.044	0.004	0.014
					0.011	0.034
ClO ₂ ⁻	0.013	0.042	0.016	0.062	0.010	0.035
	0.016	0.064	0.015	0.067	0.011	0.035
			0.01	0.038	0.014	0.046
					0.016	0.058
ClO ₃ ⁻	0.011	0.037	0.008	0.025	0.009	0.030
	0.009	0.031	0.009	0.031	0.009	0.030

			0.011	0.037	0.010 0.013	0.036 0.048
ClO ₄ ⁻	0.011 0.011	0.041 0.041	0.010 0.010 0.006	0.035 0.039 0.021	0.008 0.009 0.009 0.010	0.028 0.032 0.033 0.039

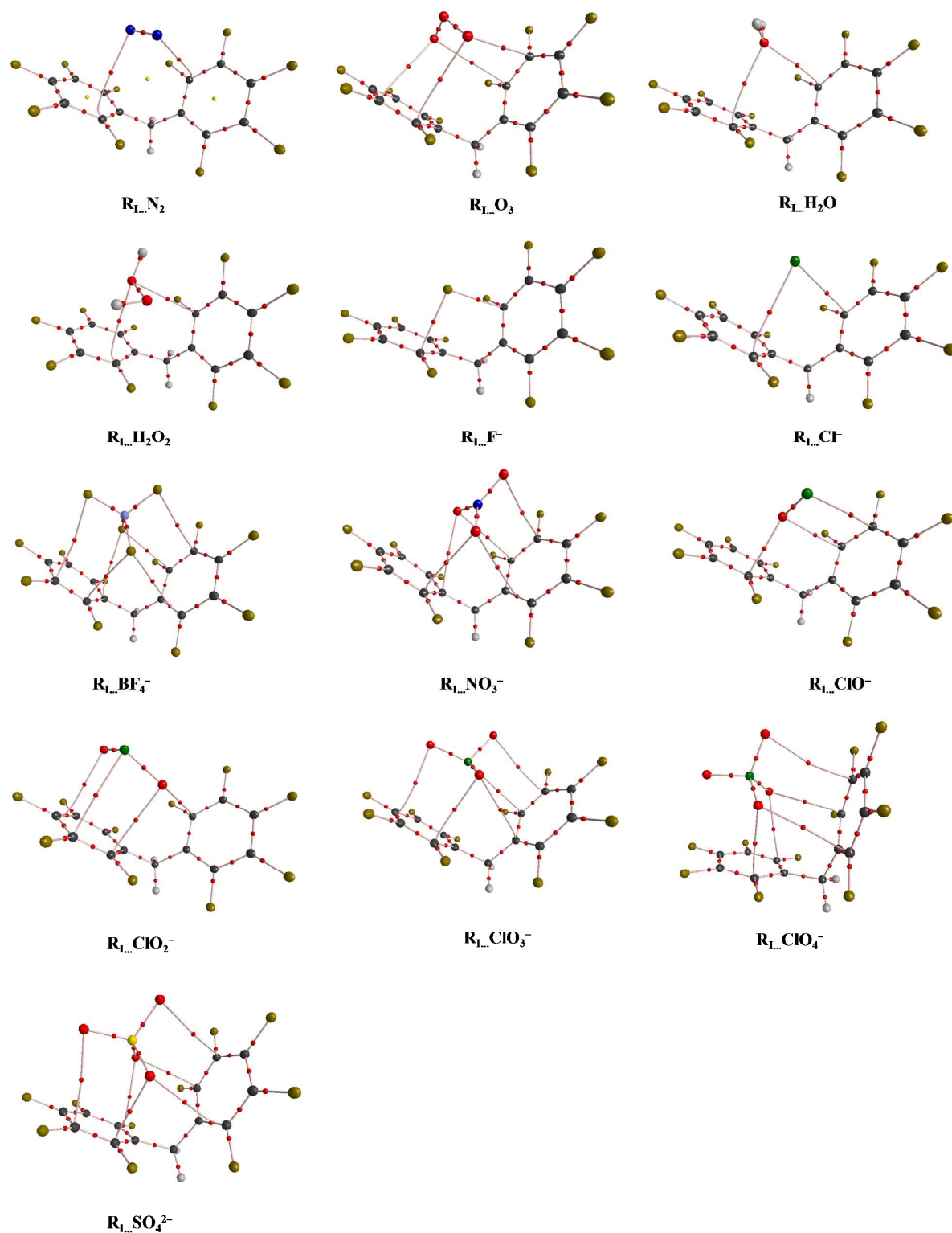


Figure S1. AIM Molecular Graphs of $R_L \cdots X$ Complexes Showing Bond Critical Points (bcps).

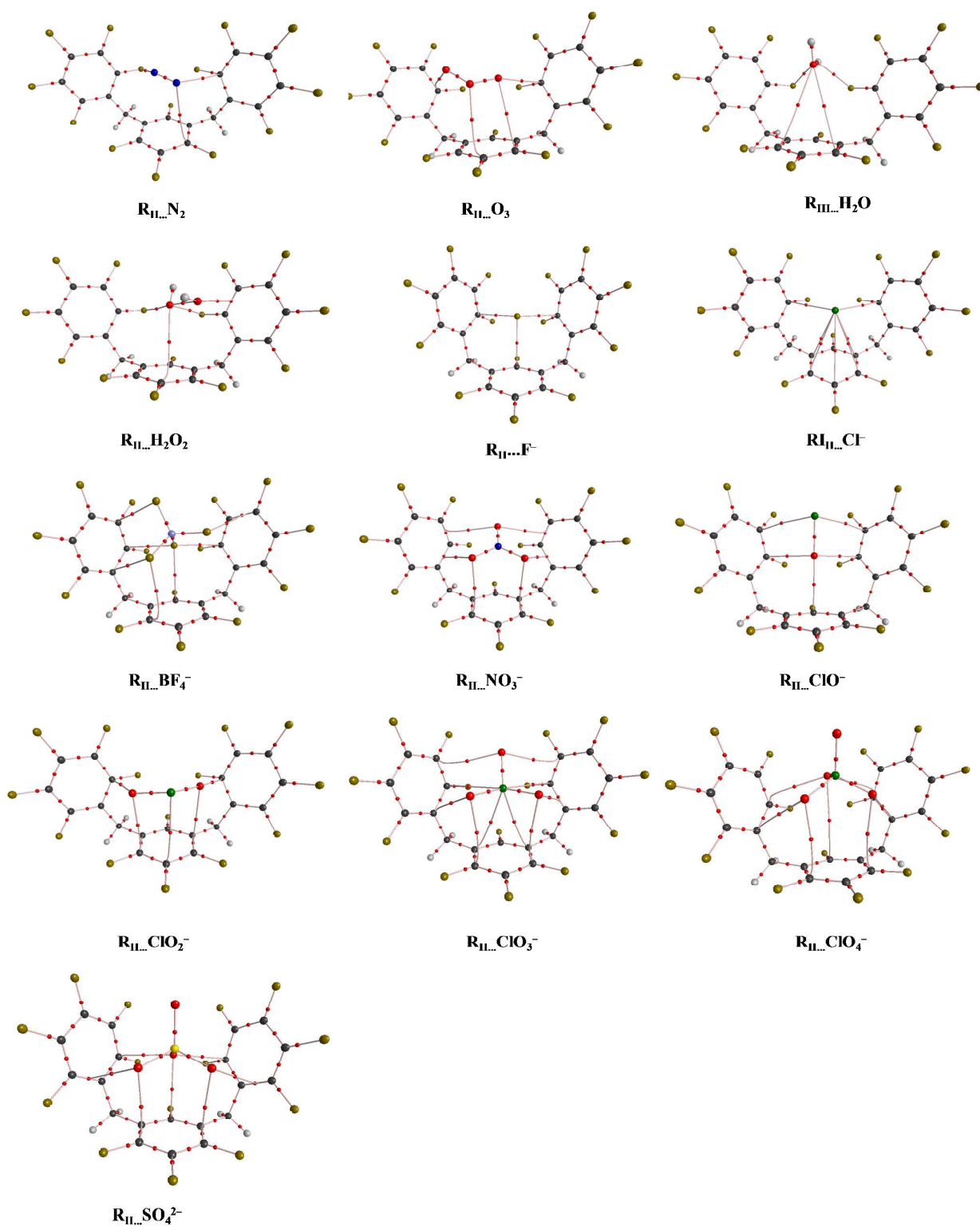


Figure S2. AIM Molecular Graphs of $\mathbf{R_I} \cdots \mathbf{X}$ Complexes Showing Bond Critical Points (bcps).

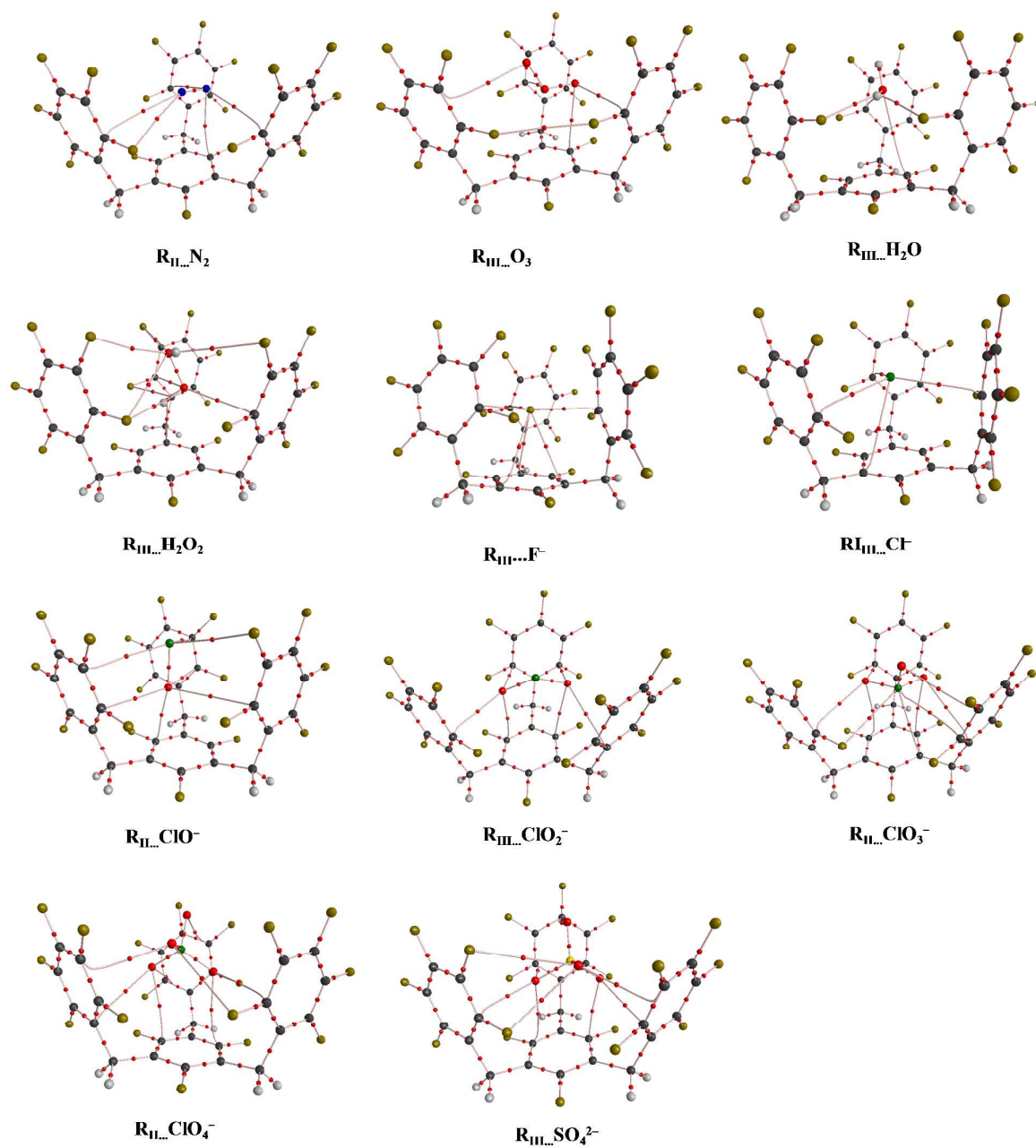


Figure S3. AIM Molecular Graphs of $R_I...X$ Complexes Showing Bond Critical Points (bcps).