

Supporting Information

**Dual Application of
(Aqua)(Chlorido)(Porphyrinato)Chromium(III) as
Hypersensitive Amine-Triggered ON Switch and for
Dioxygen Activation**

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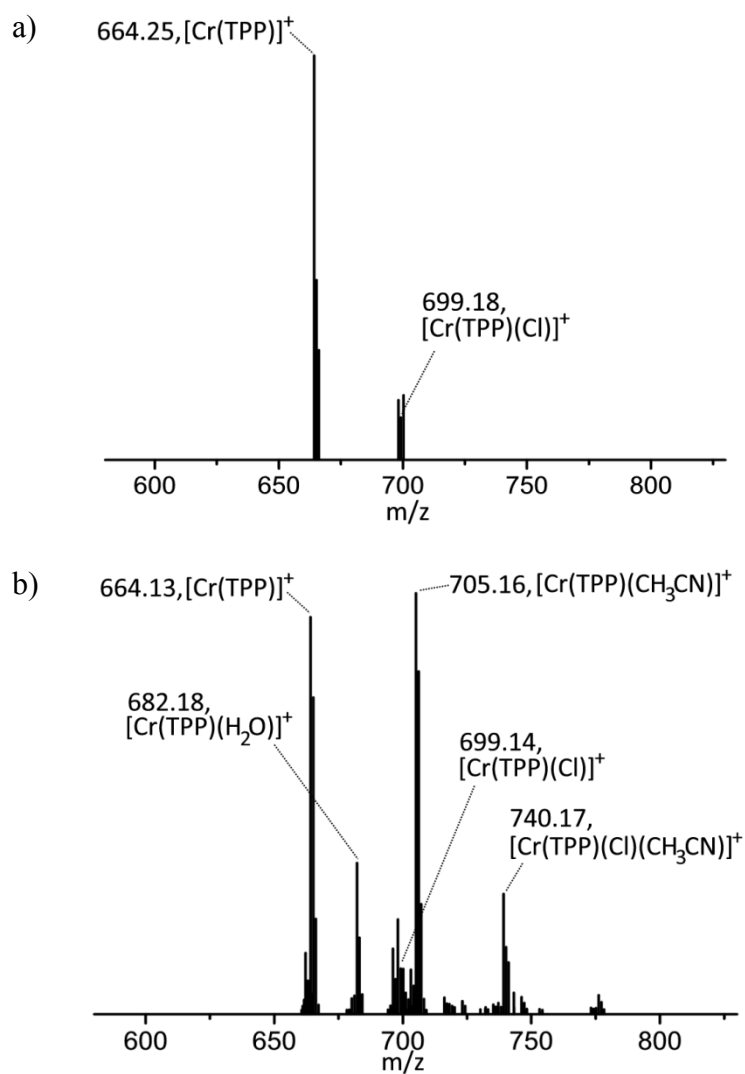


Figure S1. a) FD mass spectrum of **1**; b) ESI mass spectrum of **1**; samples were prepared in acetonitrile (CH_3CN).

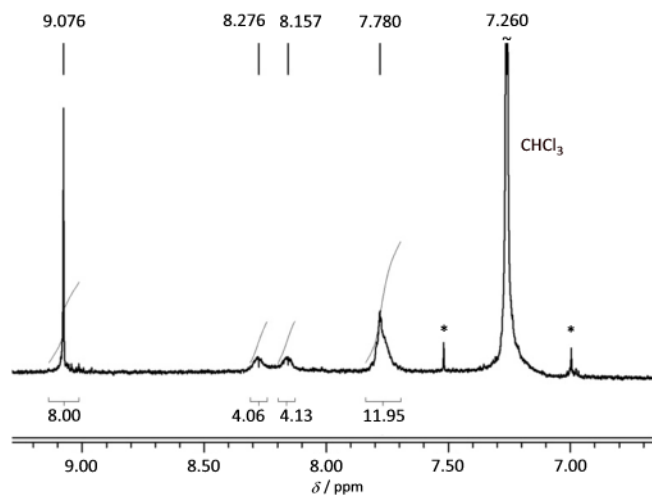


Figure S2. ^1H NMR spectrum of **4** in CDCl_3 ; sample was prepared by exposing a solution of **1** in CDCl_3 to exc. NEt_3 and air; * marks ^{13}C satellites of the solvent signal; resonances agree with literature values.⁵

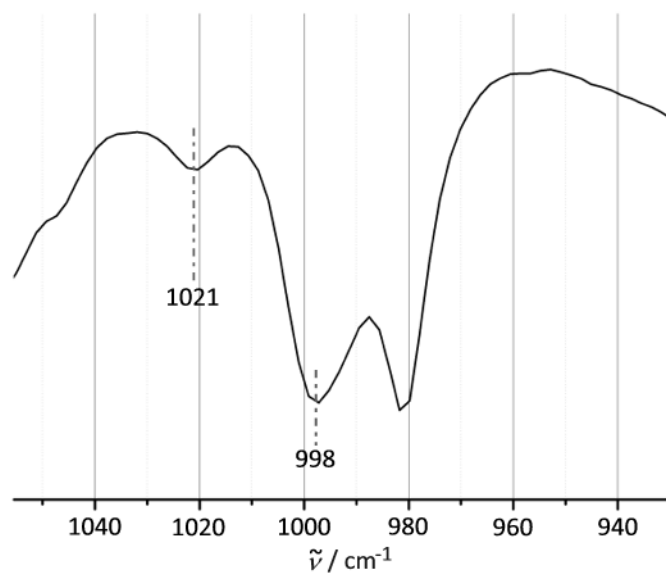


Figure S3. IR spectrum of **4** in CH_2Cl_2 ; sample was prepared by exposing a solution of **1** in CH_2Cl_2 to exc. LiOH and air; absorptions agree with literature values.⁵

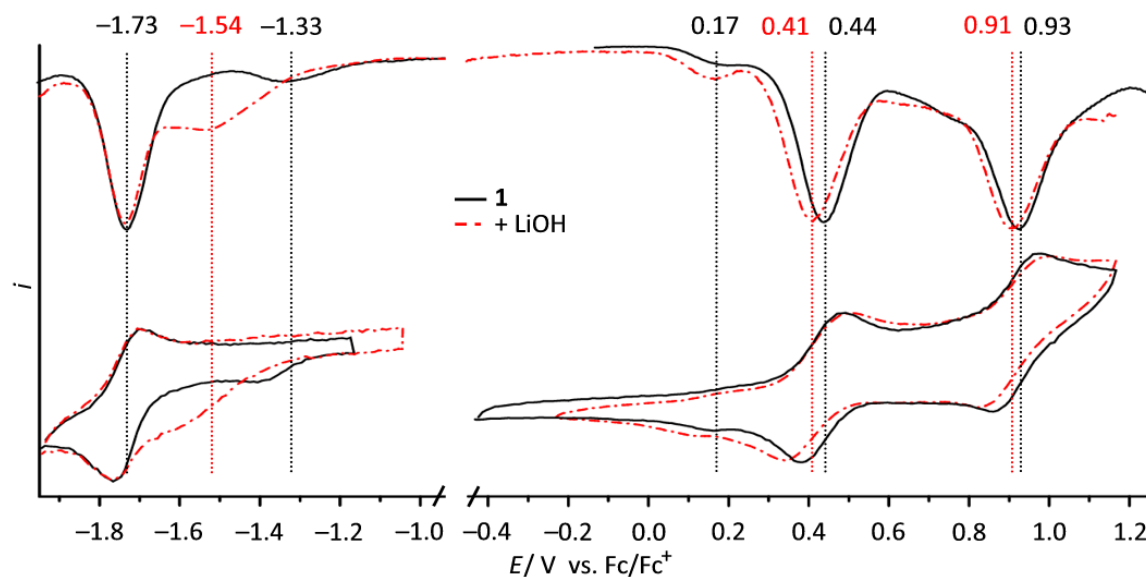


Figure S4. Square-wave voltammograms (top) and cyclic voltammograms (bottom) of **1** in CH_2Cl_2 in the absence (solid black curves) and in the presence of exc. LiOH (dashed red curves) under inert conditions.

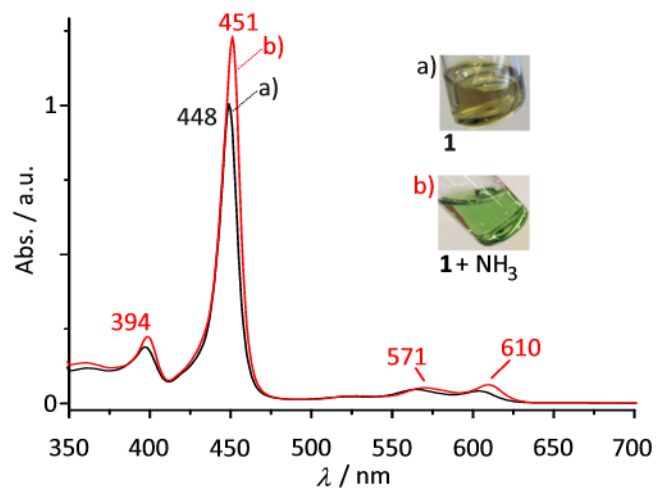


Figure S5. UV/vis absorption spectra in CH_2Cl_2 of a) **1** (black) and b) **1** with exc. NH_3 (red); insets show photographs the respective solutions.

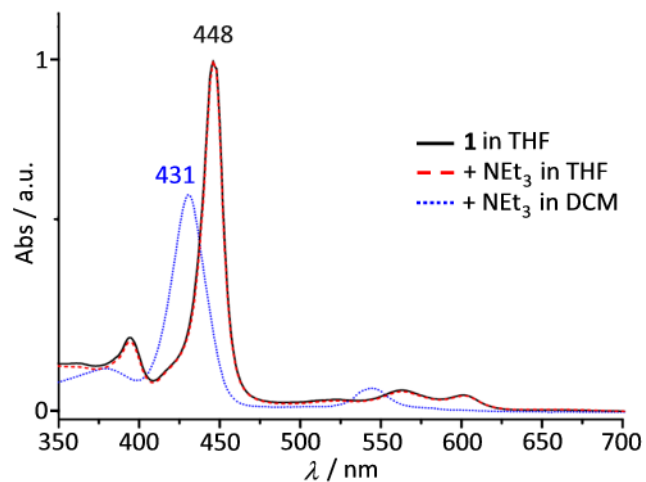


Figure S6. UV/vis spectra of a) **8** in THF (solid black curve), b) **8** in THF with exc. NEt_3 (dashed red curve) and c) **8** in CH_2Cl_2 with exc. NEt_3 exposed to moist air (dotted blue curve).

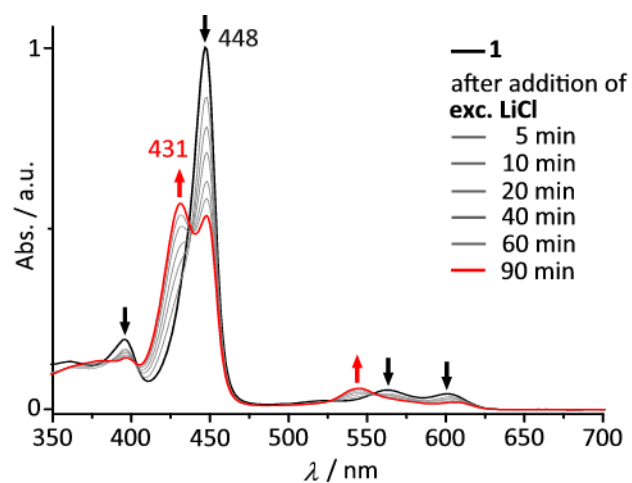


Figure S7. Temporal evolution of UV/vis absorption spectra of **1** in CH_2Cl_2 after addition of exc. LiCl ; red curve represents spectrum after 90 min.

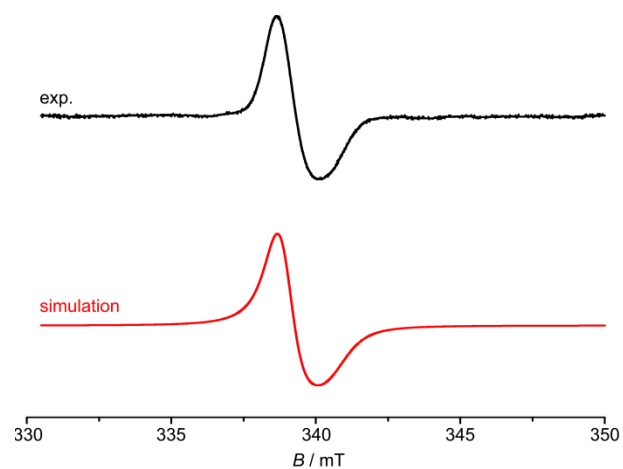


Figure S8. X-band EPR spectrum of 4^+ prepared electrochemically from **4** in $\text{CH}_2\text{Cl}_2/0.1 \text{ M } (n\text{Bu}_4\text{N})(\text{PF}_6)$ and frozen to 77 K and simulation ($g_1 = 1.9865$, $g_2 = 1.9780$).

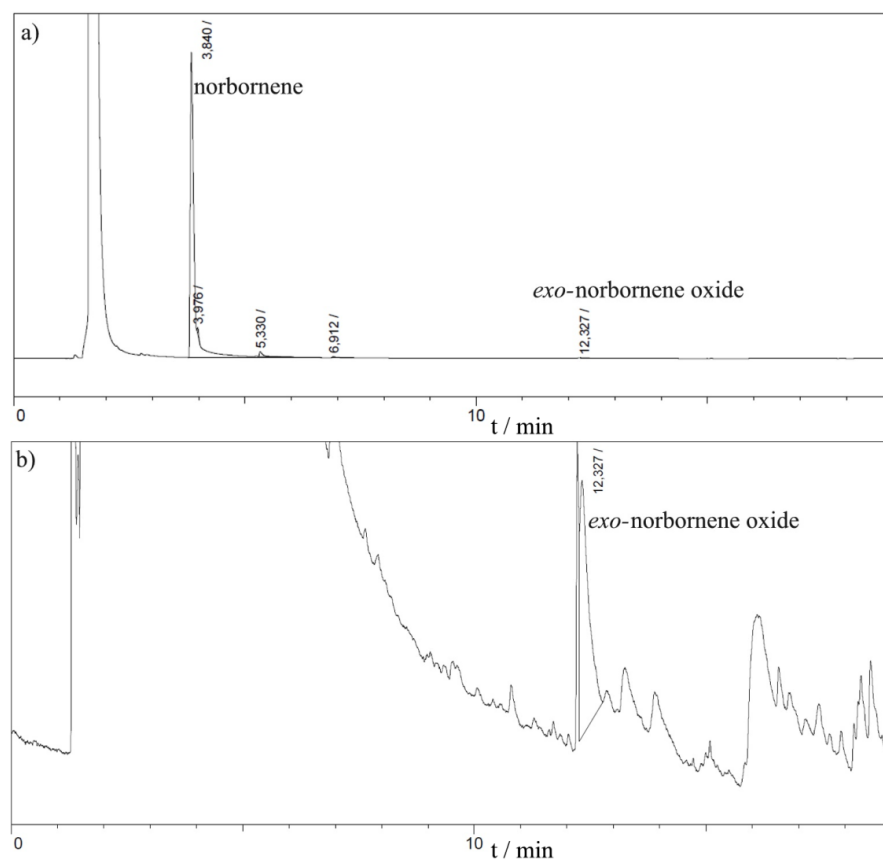


Figure S9. a) Full gas chromatogram of the electrolysis solution of **4** and 100 eq norbornene; b) magnification.

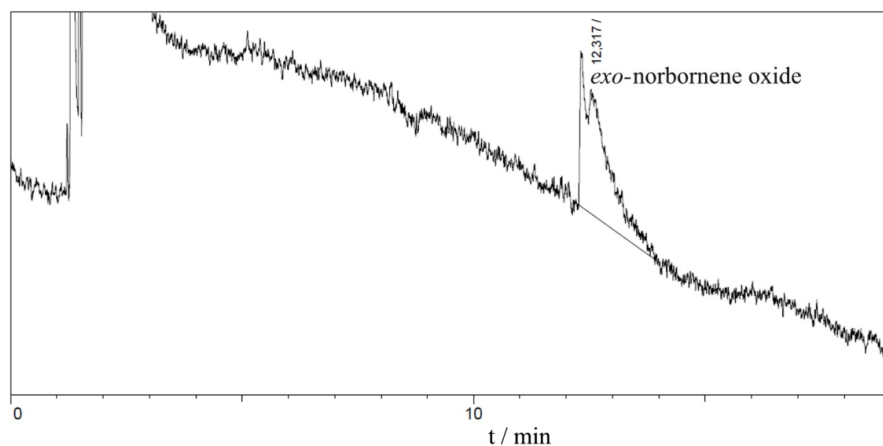


Figure S10. Gas chromatogram of an authentic sample of *exo*-norbornene oxide as received from Sigma-Aldrich at approximately the same concentration as in Figure S9 ($c = 1.8 \cdot 10^{-4} \text{ mol L}^{-1}$).

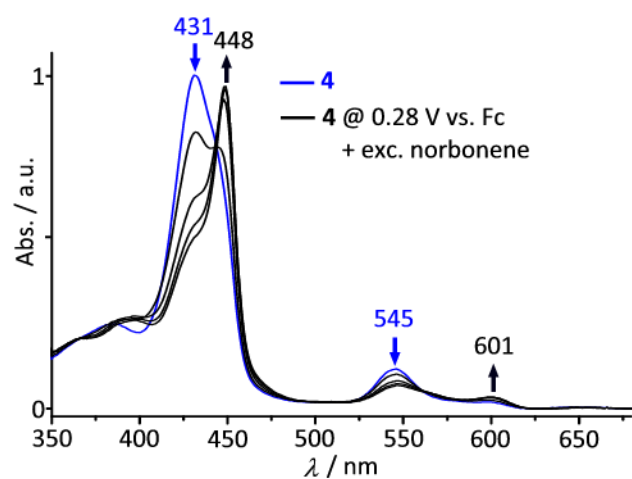
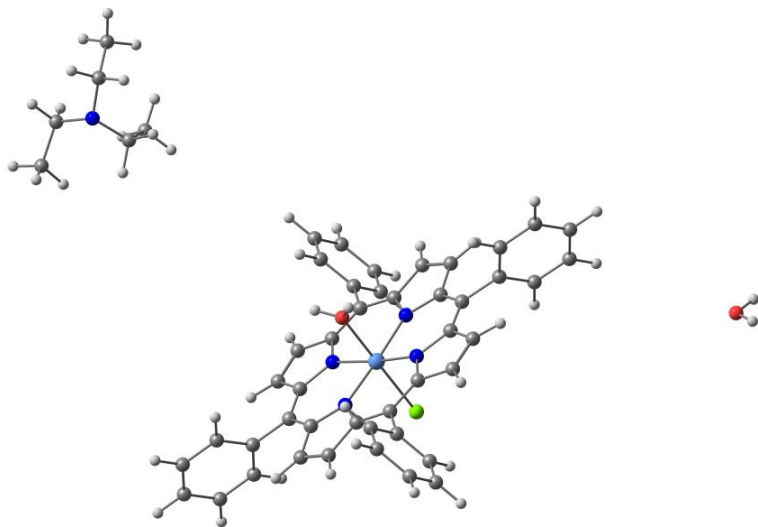


Figure S11. Spectroelectrochemical oxidation of **4** in $\text{CH}_2\text{Cl}_2/0.1 \text{ M } (n\text{Bu}_4\text{N})(\text{PF}_6)$ in the presence of norbornene.

Cartesian coordinates of optimized structures

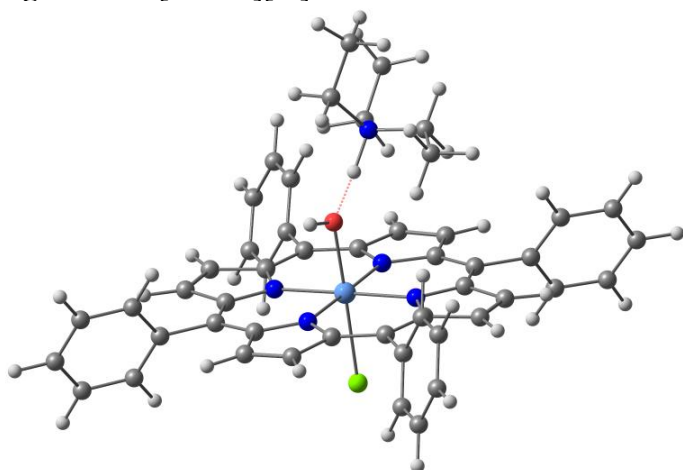
Figure S12. 1 + NEt₃ + H₂O



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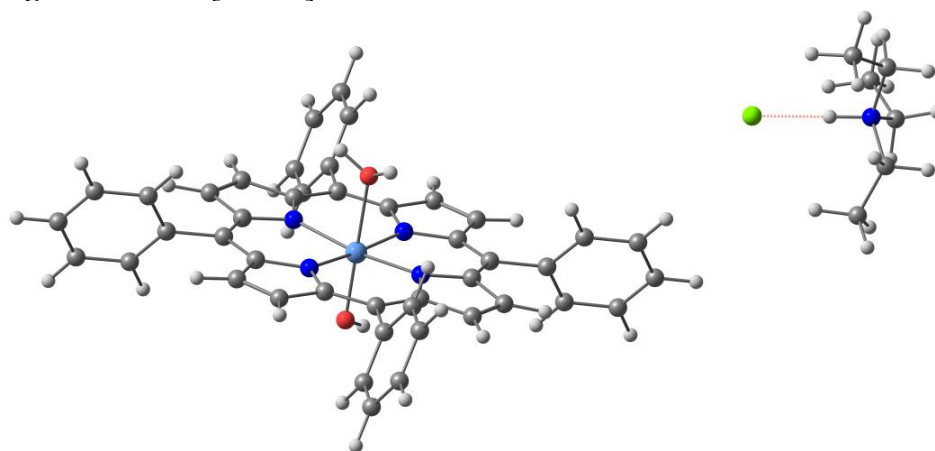
Figure S13. [HNEt₃][6⁻] + H₂O




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1	4.675412000	-4.321003000	-1.369114000
6	4.835186000	-1.436417000	-1.260351000
6	0.349375000	-3.162065000	-0.123589000
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6	5.405564000	2.155568000	-1.348800000
6	4.003002000	2.072087000	-0.970793000
6	4.758153000	-0.026190000	-1.206625000
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6	-1.261767000	0.054190000	0.248797000
6	-2.385169000	-0.841608000	0.478660000
6	-1.910013000	-2.127664000	0.386043000
6	-0.489866000	-2.044992000	0.079767000
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1	-2.466798000	-3.045001000	0.504415000
6	0.940537000	4.256559000	-0.172098000
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6	-0.254520000	2.323726000	0.009162000
6	1.793719000	3.106780000	-0.443562000
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6	3.967163000	6.701753000	-2.064916000
6	4.923835000	7.147429000	-1.130921000
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6	4.742756000	5.015097000	0.045397000
1	3.666805000	7.346126000	-2.887479000
1	6.044087000	6.633339000	0.654070000
6	6.648636000	-1.893278000	-2.970970000
1	-0.227670000	-7.291536000	2.042386000
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1	8.236416000	-2.347918000	-4.367623000
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1	0.772100000	-5.022316000	1.839017000
1	-1.834776000	-8.115296000	0.310505000
1	5.042219000	4.368534000	0.866742000
1	5.362041000	8.137901000	-1.225570000
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7	4.154355000	0.092414000	3.031548000
6	3.507307000	0.273027000	4.401728000
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6	4.915168000	-1.209554000	2.867659000
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1	5.368946000	-1.172210000	1.871640000
6	4.957694000	1.297152000	2.559184000
1	5.195956000	1.099917000	1.509412000
1	4.269956000	2.149626000	2.584380000
6	6.240672000	1.621339000	3.337387000
1	6.758138000	2.436581000	2.816840000
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1	3.205565000	-2.405386000	2.235949000
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1	3.762452000	0.118934000	6.526552000
1	5.285109000	0.460494000	5.694442000
1	4.591224000	-1.173980000	5.654915000
8	-91.117752000	-0.083832000	-0.400740000
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1	-91.583536000	0.774072000	-0.356647000

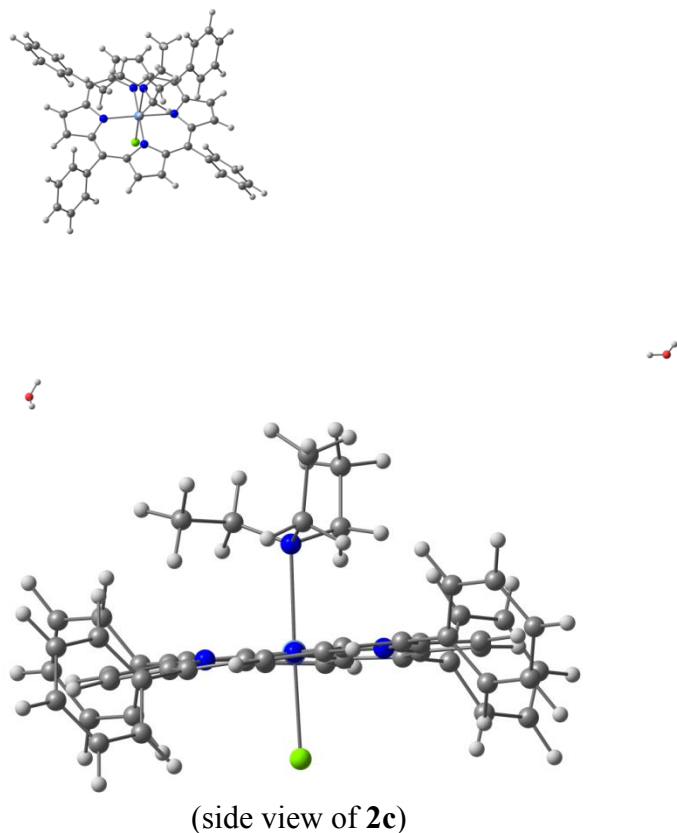
Figure S14. 7 + [HNEt₃]Cl



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6	-7.166564000	-3.024473000	-0.149268000
6	-6.072389000	-3.939625000	-0.438634000
6	-4.949644000	-3.179653000	-0.659995000
6	-5.333843000	-1.783611000	-0.511330000
1	-6.159481000	-5.014526000	-0.489253000
1	-3.961851000	-3.526625000	-0.923589000
6	-4.462722000	-0.691277000	-0.720478000
6	-8.500509000	-3.426776000	0.083724000
6	-3.959932000	1.794383000	-0.822505000
6	-4.706397000	2.938162000	-0.673249000
6	-6.078036000	2.529943000	-0.408551000
6	-4.862227000	0.662973000	-0.665552000
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6	-9.567431000	3.938294000	0.382496000
6	-10.689773000	3.177452000	0.604473000
6	-10.300845000	1.780687000	0.473029000
6	-8.469076000	3.022633000	0.110343000
1	-9.485786000	5.014596000	0.409120000
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6	-11.180762000	0.687964000	0.634074000
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6	-2.183901000	-1.579495000	-0.051182000
6	-0.832868000	-1.855632000	-0.334932000
6	-0.298769000	-1.552589000	-1.603461000
6	-1.126237000	-0.968606000	-2.583571000
6	-8.796507000	-4.900796000	0.106540000
6	-9.582321000	-5.493363000	-0.908995000
6	-9.856368000	-6.874080000	-0.892900000
6	-8.572466000	-7.103400000	1.163265000
6	-8.293447000	-5.723541000	1.140822000
1	-10.456324000	-7.313097000	-1.686202000
6	-12.626350000	0.986804000	0.923096000
6	-13.453856000	1.561666000	-0.068919000
6	-14.808276000	1.839260000	0.197213000
6	-15.355452000	1.552228000	1.463914000
6	-14.537812000	0.982534000	2.460474000
6	-13.185323000	0.699647000	2.189697000
6	-6.851109000	4.899546000	-0.208749000
6	-7.342163000	5.702994000	-1.263320000

6	-7.067781000	7.083511000	-1.303326000
6	-6.301993000	7.683779000	-0.283768000
6	-5.811219000	6.891787000	0.773652000
6	-6.081502000	5.510378000	0.807945000
1	-7.448515000	7.684732000	-2.125287000
1	-5.222318000	7.345565000	1.567007000
6	-2.474932000	-0.686520000	-2.294925000
1	-8.182586000	-7.719010000	1.970206000
1	-3.109426000	-0.243259000	-3.058503000
1	-0.202330000	-2.303364000	0.429320000
1	-0.725765000	-0.735563000	-3.567097000
1	-12.559241000	0.264708000	2.965186000
1	-14.948995000	0.760228000	3.442128000
1	-15.431341000	2.275273000	-0.579792000
7	-8.936116000	1.710511000	0.190257000
6	-9.354397000	-7.684738000	0.145013000
1	-16.400665000	1.768605000	1.670631000
1	0.743611000	-1.768428000	-1.824486000
1	-9.966555000	-4.875079000	-1.716445000
1	-7.693340000	-5.281509000	1.932644000
1	-9.568159000	-8.750604000	0.159690000
1	-5.703387000	4.906128000	1.629144000
1	-6.091366000	8.749977000	-0.312802000
1	-7.929606000	5.245349000	-2.055621000
1	-13.039330000	1.779651000	-1.050138000
1	-2.587693000	-1.810574000	0.931655000
24	-7.841268000	-0.002179000	-0.148317000
8	-8.206922000	-0.060273000	-1.994296000
1	-7.561044000	0.442100000	-2.535008000
7	37.943438000	-0.269538000	0.246282000
6	38.920226000	0.678501000	-0.449288000
1	38.725128000	0.601599000	-1.520979000
1	39.929127000	0.296544000	-0.255363000
6	38.769575000	2.140676000	-0.004621000
1	39.047943000	2.297005000	1.042955000
1	39.435508000	2.758595000	-0.618323000
1	37.740874000	2.486780000	-0.150547000
6	38.331559000	-0.481259000	1.709391000
1	38.590257000	0.500814000	2.111218000
1	39.234030000	-1.103091000	1.714593000
6	37.210032000	-1.100593000	2.555546000
1	37.541975000	-1.128754000	3.600050000
1	36.299194000	-0.495614000	2.497025000
1	36.970369000	-2.127203000	2.258937000
6	37.841223000	-1.600023000	-0.499715000
1	38.864322000	-1.965814000	-0.643411000
1	37.318627000	-2.294030000	0.161896000
6	37.083868000	-1.492692000	-1.831216000
1	37.607847000	-0.876719000	-2.569859000
1	36.983541000	-2.499541000	-2.253242000
1	36.082022000	-1.078785000	-1.675959000
1	36.974114000	0.189478000	0.229019000
17	35.159902000	1.045621000	0.195860000
8	-7.425530000	0.038011000	1.958783000
1	-7.988615000	0.572001000	2.550440000
1	-7.115128000	-0.781700000	2.387827000

Figure S15. 2c + 2 H₂O



7	-1.891580000	-1.078689000	1.478480000
7	-2.103620000	-0.729862000	-1.388675000
7	0.872035000	-0.194785000	1.372659000
6	-1.635728000	-1.041713000	2.852353000
6	-2.832122000	-1.445229000	3.572071000
6	-3.798566000	-1.727273000	2.637200000
6	-3.223858000	-1.466958000	1.327307000
1	-2.919305000	-1.501580000	4.646565000
1	-4.809706000	-2.060221000	2.815508000
6	-3.940656000	-1.537424000	0.114488000
6	-0.418087000	-0.682168000	3.467033000
6	-4.200704000	-1.018258000	-2.346656000
6	-3.375785000	-0.511577000	-3.321238000
6	-2.060962000	-0.335865000	-2.727466000
6	-3.410835000	-1.142588000	-1.132561000
1	-5.250964000	-1.254602000	-2.428338000
1	-3.632385000	-0.265273000	-4.340509000
6	-0.936403000	0.156874000	-3.420758000
6	2.186903000	0.200173000	1.119423000
6	2.911483000	0.282617000	2.377264000
6	2.023504000	-0.018538000	3.381717000
6	0.743370000	-0.308997000	2.757243000
1	3.955330000	0.539286000	2.476043000
1	2.217109000	-0.053799000	4.443254000
6	1.497786000	0.844955000	-3.538750000
6	2.522950000	0.934162000	-2.628379000
6	2.000542000	0.498642000	-1.344114000
6	0.328232000	0.354979000	-2.827712000
1	1.526121000	1.091964000	-4.589257000
1	3.531471000	1.277577000	-2.802468000
6	2.738866000	0.510568000	-0.141675000
6	-5.372661000	-1.994614000	0.153876000

6	-5.739637000	-3.237416000	-0.411523000
6	-7.078393000	-3.672752000	-0.383706000
6	-8.073157000	-2.865542000	0.203436000
6	-7.717876000	-1.621593000	0.762887000
6	-0.348825000	-0.700726000	4.968957000
6	-0.253430000	0.508387000	5.695394000
6	-0.190135000	0.498176000	7.101862000
6	-0.304455000	-1.934397000	7.087667000
6	-0.375053000	-1.921463000	5.681515000
1	-0.123874000	1.437748000	7.644768000
6	4.181606000	0.929169000	-0.204798000
6	4.600543000	2.163635000	0.342594000
6	5.950146000	2.558238000	0.274835000
6	6.904056000	1.720400000	-0.337125000
6	6.496153000	0.487727000	-0.885020000
6	5.144499000	0.098343000	-0.822563000
6	-1.097428000	0.507668000	-4.874313000
6	-1.069889000	1.858354000	-5.291457000
6	-1.224456000	2.193666000	-6.649952000
6	-1.401866000	1.181285000	-7.614314000
6	-1.427006000	-0.168004000	-7.208492000
6	-1.279511000	-0.500726000	-5.848202000
1	-1.207504000	3.237862000	-6.952154000
1	-1.560025000	-0.956747000	-7.944877000
6	-6.377573000	-1.191414000	0.740161000
1	-0.319916000	-2.882540000	7.619541000
1	-6.111883000	-0.226492000	1.164768000
1	-7.342114000	-4.634134000	-0.817611000
1	-8.478989000	-0.988304000	1.211879000
1	4.837362000	-0.855224000	-1.245384000
1	7.224411000	-0.166527000	-1.357939000
1	6.253398000	3.513912000	0.695121000
7	0.662731000	0.130252000	-1.492214000
6	-0.213765000	-0.723844000	7.803580000
1	7.946889000	2.023571000	-0.387315000
1	-9.107817000	-3.198801000	0.222494000
1	-0.240070000	1.454376000	5.159677000
1	-0.440077000	-2.859767000	5.135725000
1	-0.162764000	-0.732671000	8.889519000
1	-1.294990000	-1.544375000	-5.543432000
1	-1.518721000	1.439532000	-8.663886000
1	-0.939160000	2.644029000	-4.551463000
1	3.868210000	2.818217000	0.808534000
1	-4.976526000	-3.865554000	-0.865022000
17	-1.333785000	1.802171000	0.304469000
7	0.153983000	-2.840468000	-0.254506000
6	1.385535000	-2.829224000	-1.133427000
1	2.076385000	-2.107657000	-0.690958000
1	1.082700000	-2.425405000	-2.101367000
6	-0.952005000	-3.723030000	-0.806275000
1	-0.752658000	-4.762815000	-0.519723000
1	-1.874422000	-3.422956000	-0.300451000
6	0.496299000	-3.267502000	1.169076000
1	-0.257542000	-2.830320000	1.821476000
1	1.452513000	-2.794033000	1.408850000
24	-0.604502000	-0.500696000	-0.012856000
6	0.570204000	-4.775893000	1.512611000
1	0.983242000	-4.857562000	2.527326000
1	-0.418749000	-5.247779000	1.529672000
1	1.215878000	-5.352440000	0.845711000
6	-1.149788000	-3.702416000	-2.330442000
1	-0.323428000	-4.191673000	-2.858133000
1	-2.064736000	-4.262028000	-2.565100000
1	-1.263745000	-2.693372000	-2.725148000
6	2.137107000	-4.162376000	-1.347374000
1	2.882854000	-4.011772000	-2.139595000
1	2.674251000	-4.483251000	-0.448958000
1	1.476226000	-4.976331000	-1.665955000
8	34.827108000	5.321344000	0.205190000
1	35.364454000	4.517200000	0.345004000
1	34.133465000	5.134199000	-0.457205000

8	-12.352025000	24.229164000	1.792373000
1	-11.688529000	24.205295000	1.075397000
1	-12.129790000	23.550826000	2.459738000