ELECTRONIC SUPPLEMENTARY INFORMATION

Corresponding to the Manuscript:

Exploring Protonation Sites with Cation-Responsive Polyethylene glycol (PEG) Tethers in [FeFe]-Hydrogenase Mimics

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S1. NMR

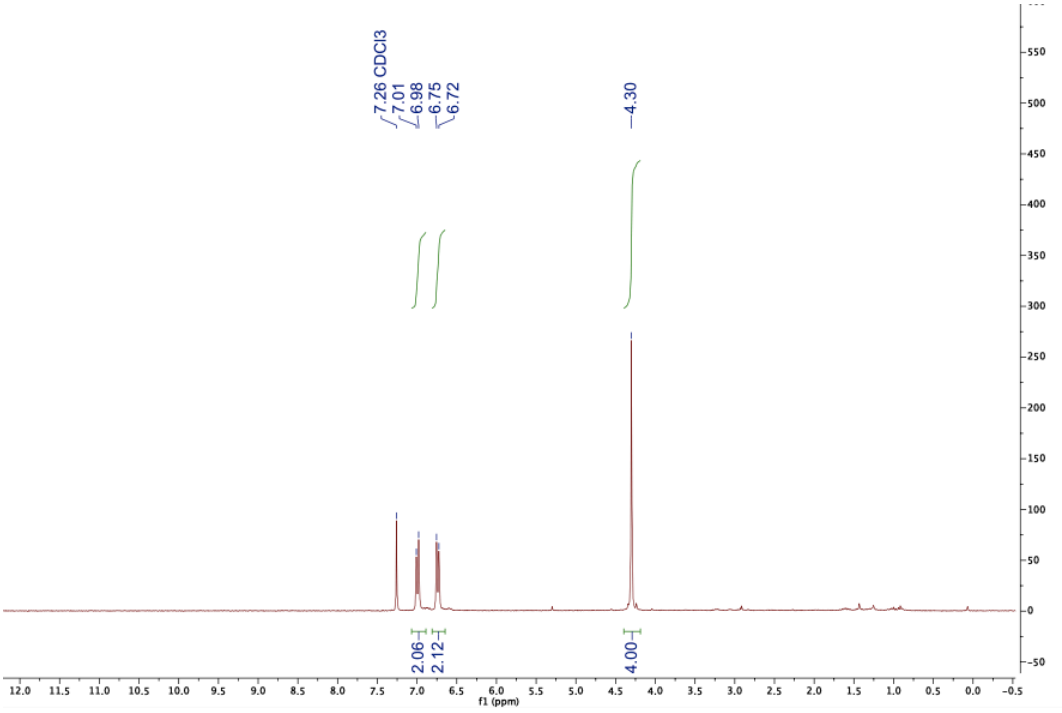

Figure S1. ^{1}H-NMR (300 MHz) of compound **11** in $CDCl_3$.

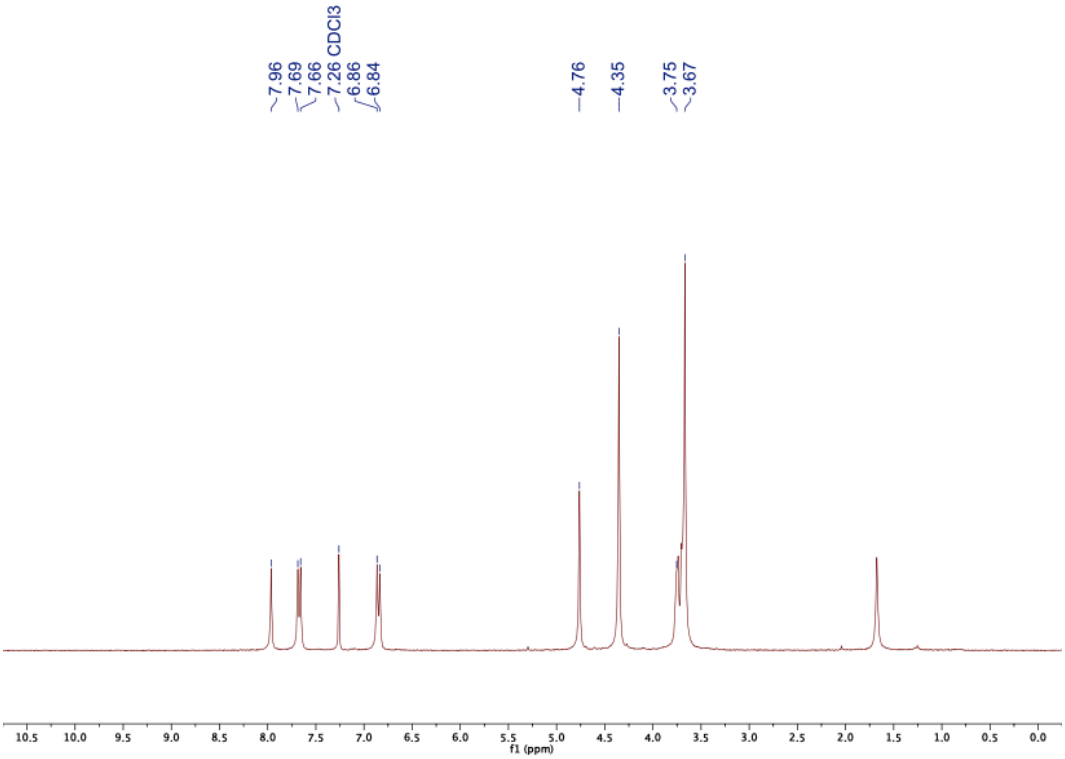

Figure S2. ^{1}H-NMR (500 MHz) of compound **7** in $CDCl_3$.

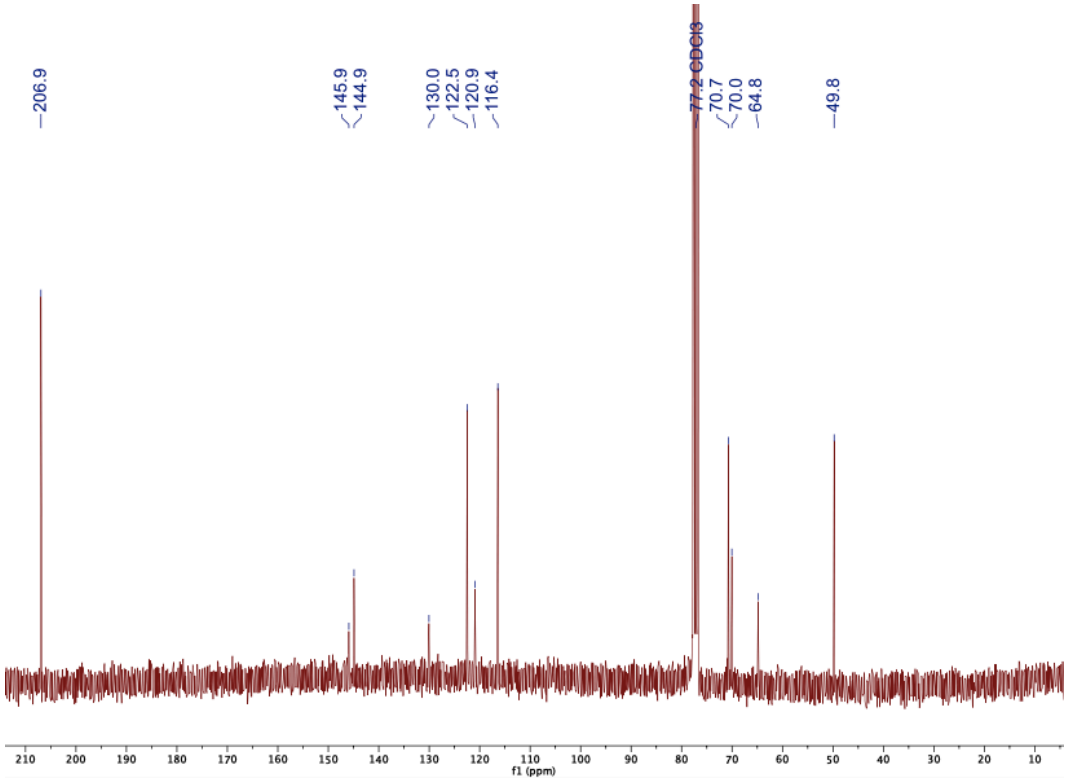

Figure S3. $^{13}C\{^{1}H\}$-NMR (126 MHz) of compound **7** in $CDCl_3$.

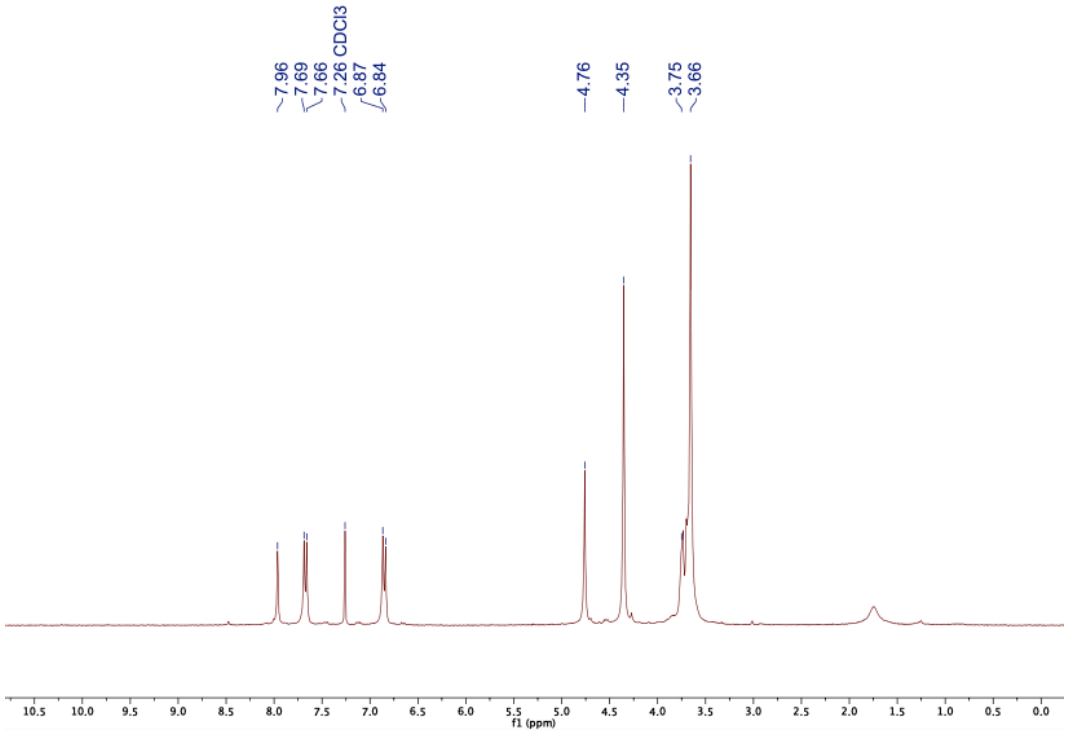

Figure S4. ^{1}H-NMR (500 MHz) of compound **8** in $CDCl_3$.

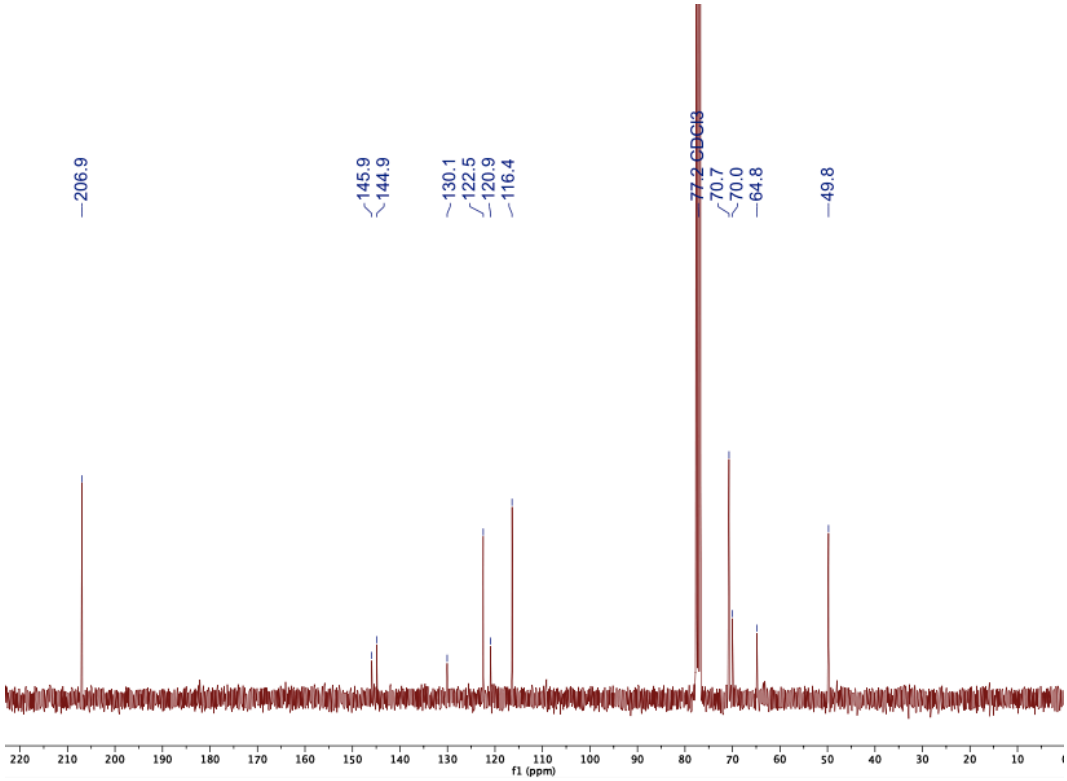

Figure S5. $^{13}C\{^{1}H\}$-NMR (126 MHz) of compound **8** in $CDCl_3$.

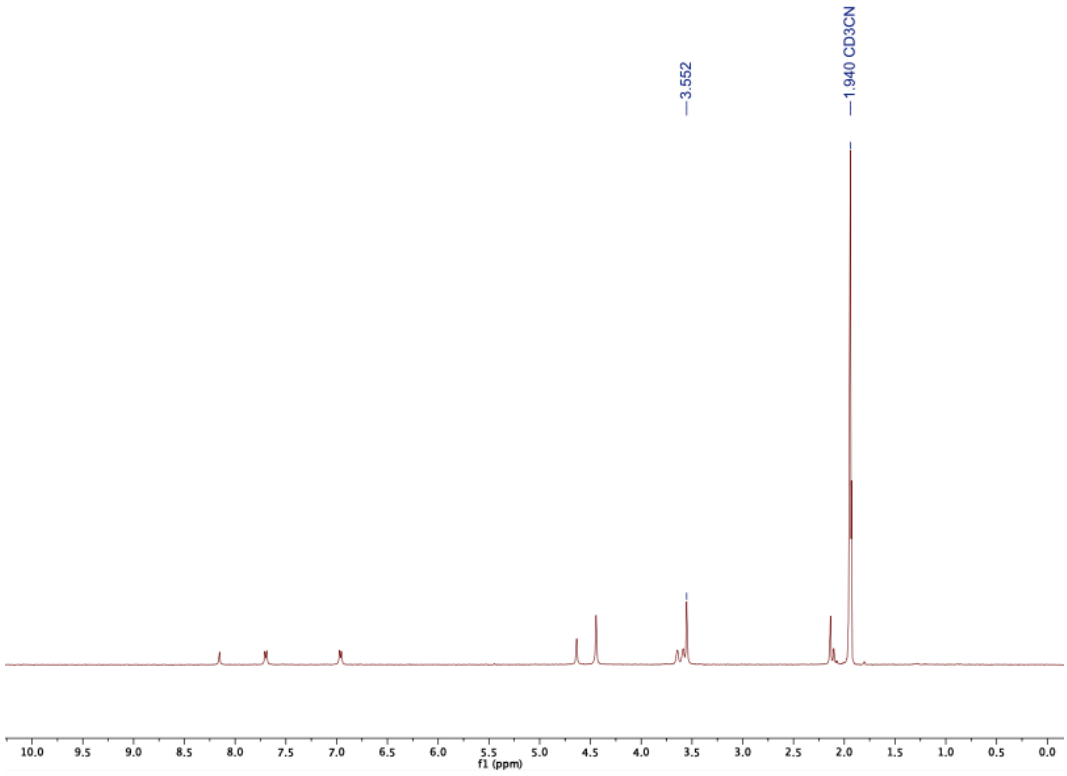

Figure S6. ^{1}H-NMR (500 MHz) of compound **7** + 0 equiv. of $NaPF_6$ in CD_3CN.

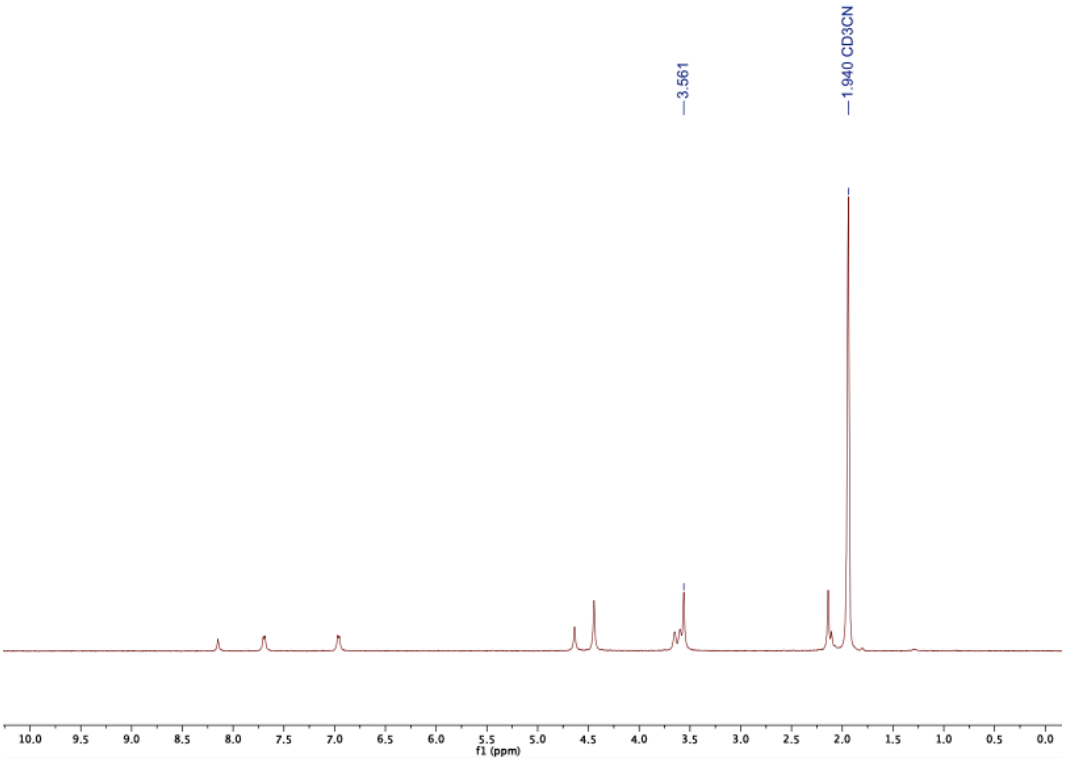

Figure S7. ^{1}H-NMR (500 MHz) of compound **7** + 0.1 equiv. of $NaPF_6$ in CD_3CN.

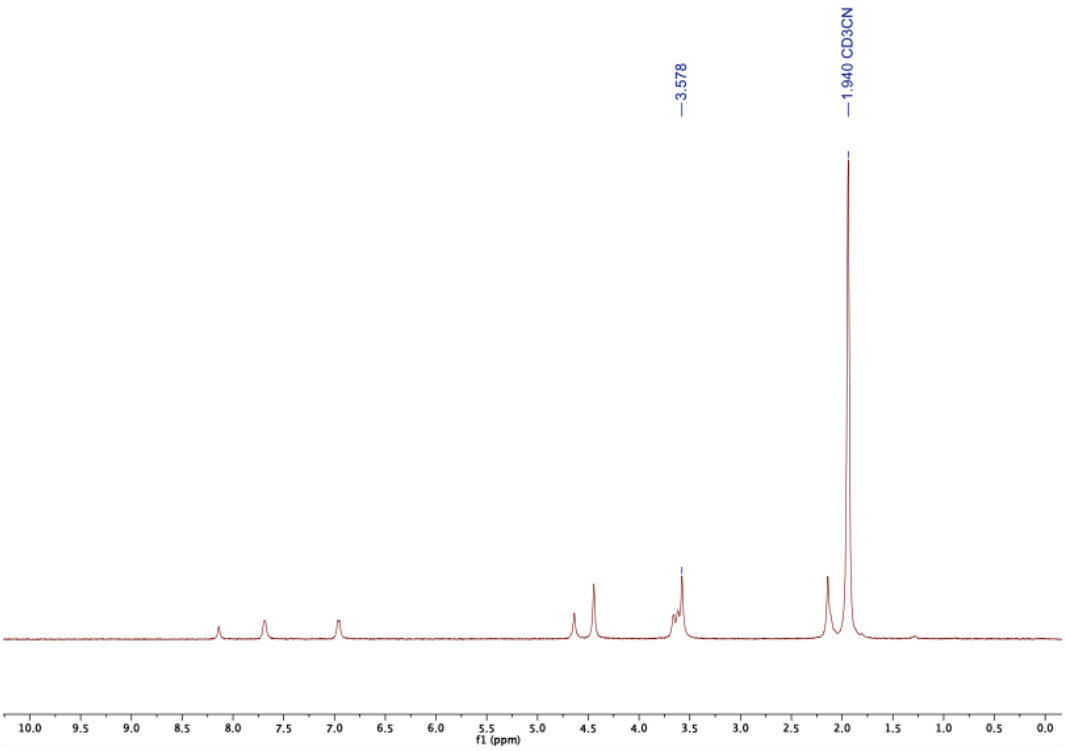

Figure S8. ^{1}H-NMR (500 MHz) of compound **7** + 0.3 equiv. of $NaPF_6$ in CD_3CN.

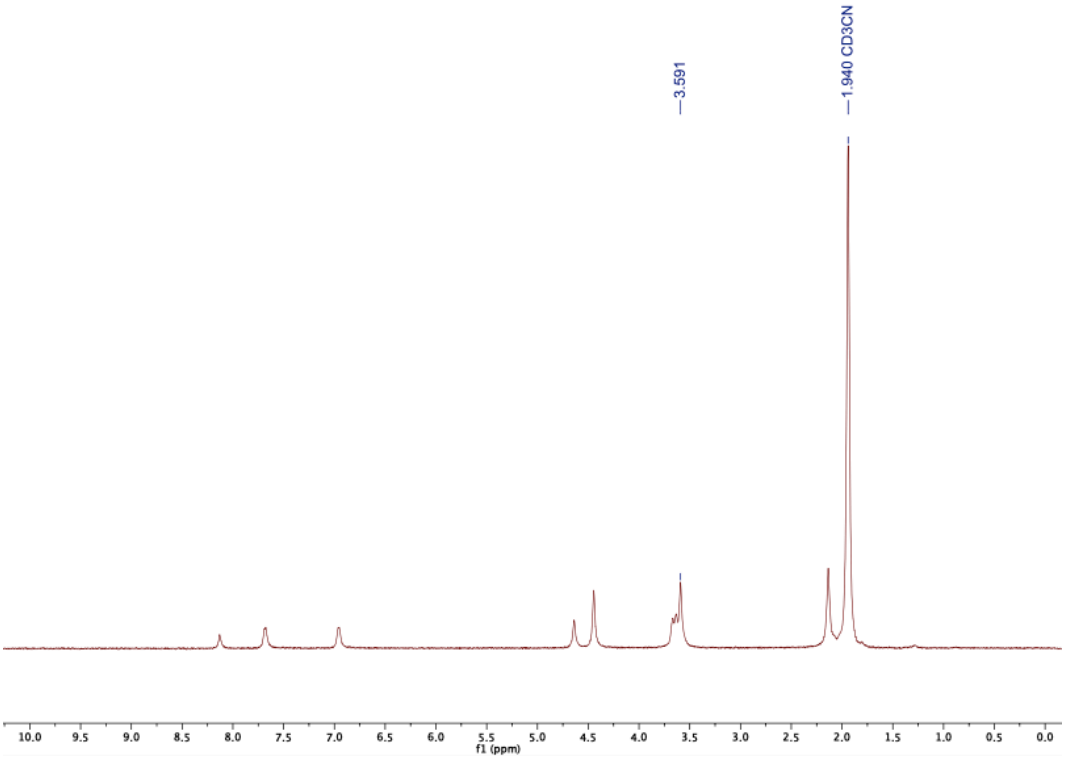

Figure S9. ^{1}H-NMR (500 MHz) of compound **7** + 0.5 equiv. of $NaPF_6$ in CD_3CN.

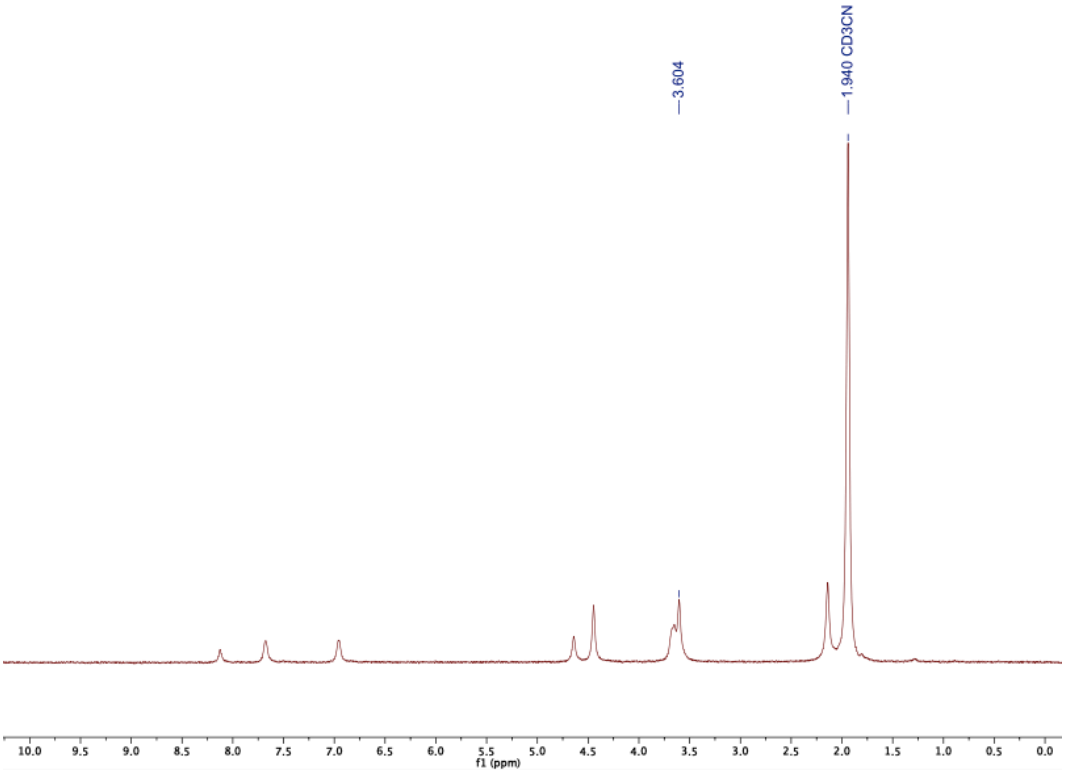

Figure S10. ^{1}H-NMR (500 MHz) of compound **7** + 0.7 equiv. of $NaPF_6$ in CD_3CN.

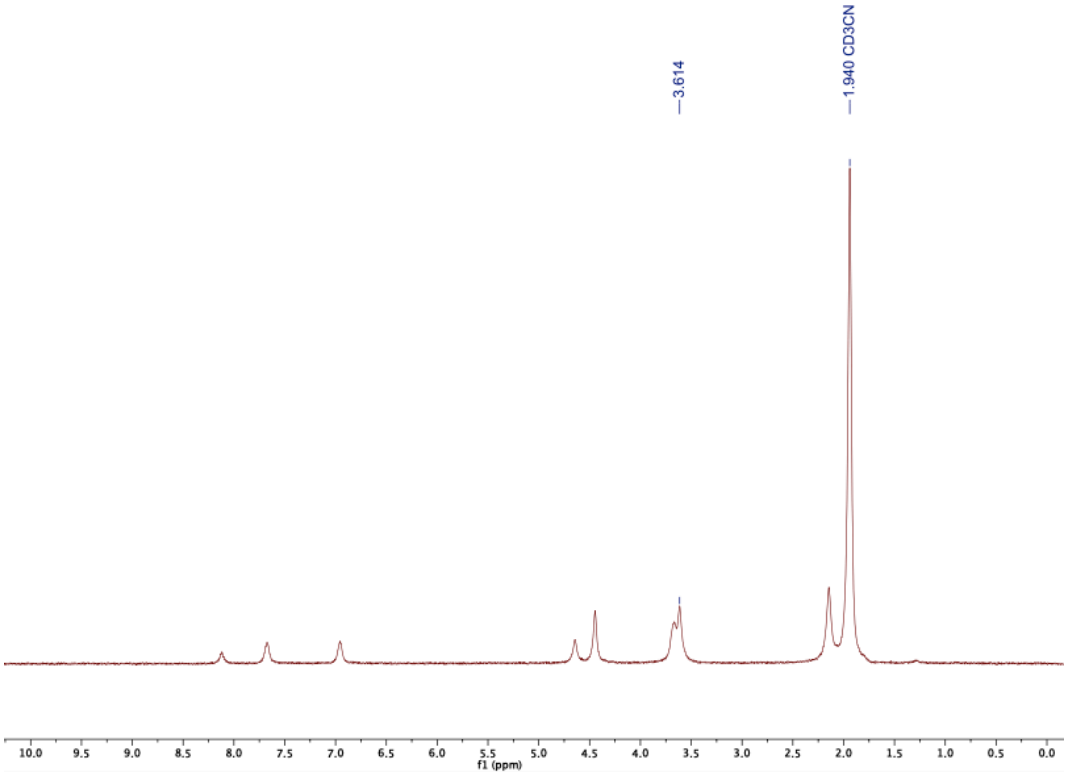

Figure S11. ^{1}H-NMR (500 MHz) of compound **7** + 0.9 equiv. of $NaPF_6$ in CD_3CN.

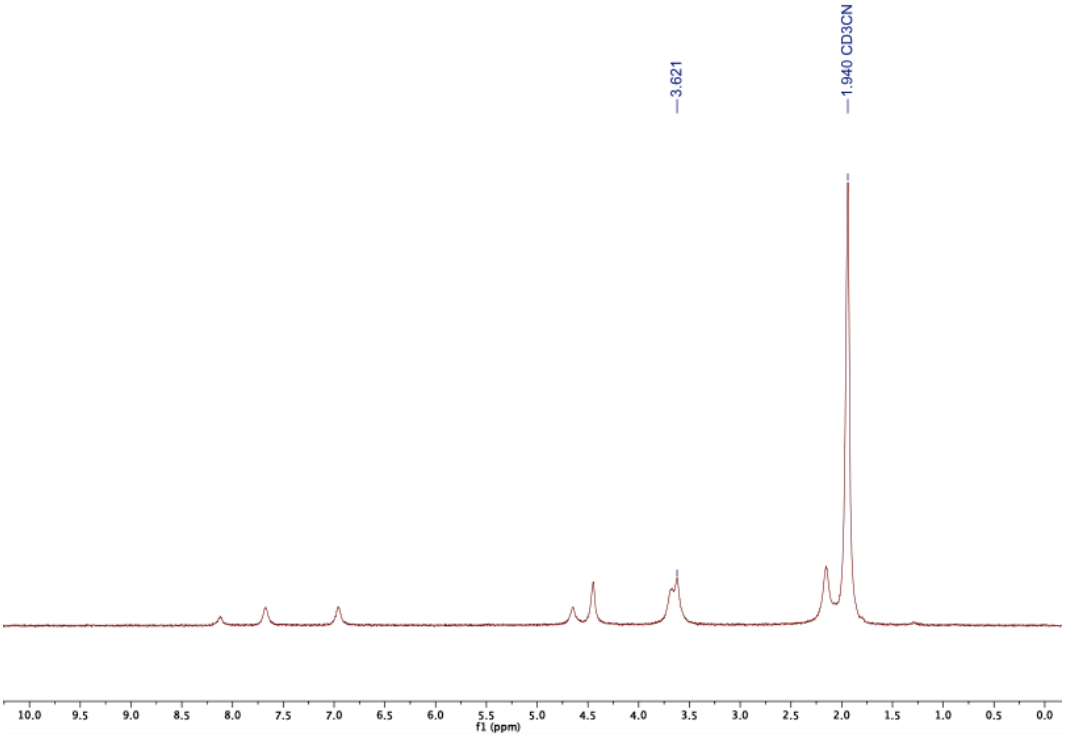

Figure S12. ^{1}H-NMR (500 MHz) of compound **7** + 1 equiv. of $NaPF_6$ in CD_3CN.

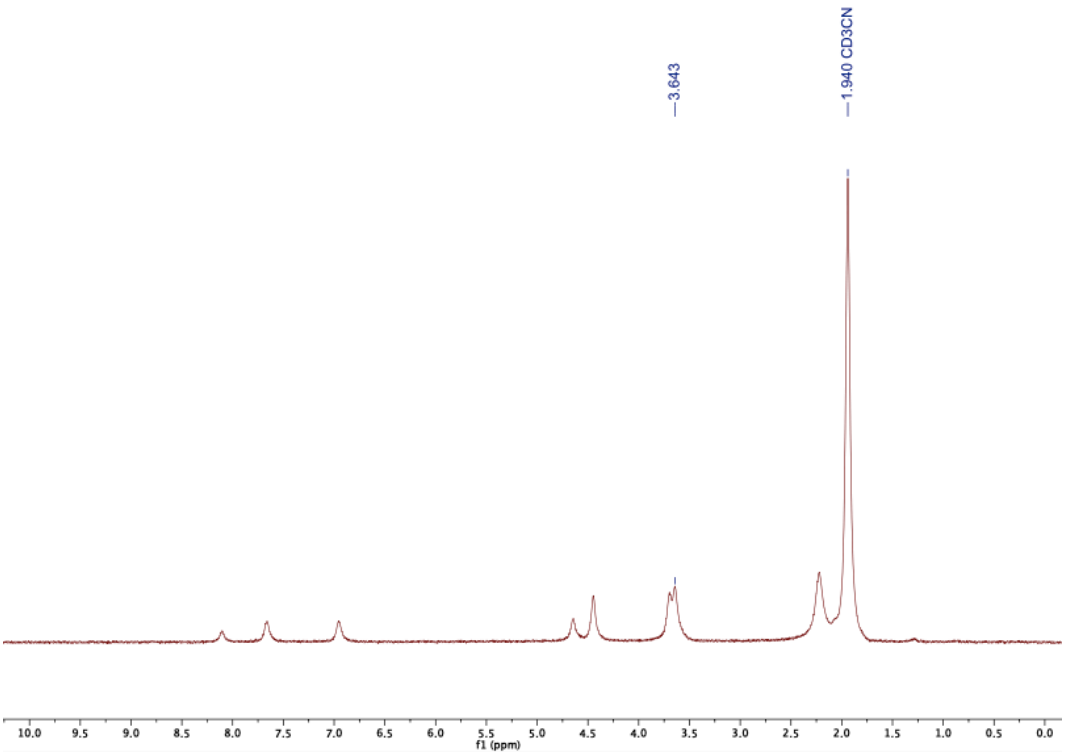

Figure S13. ^{1}H-NMR (500 MHz) of compound **7** + 2 equiv. of $NaPF_6$ in CD_3CN.

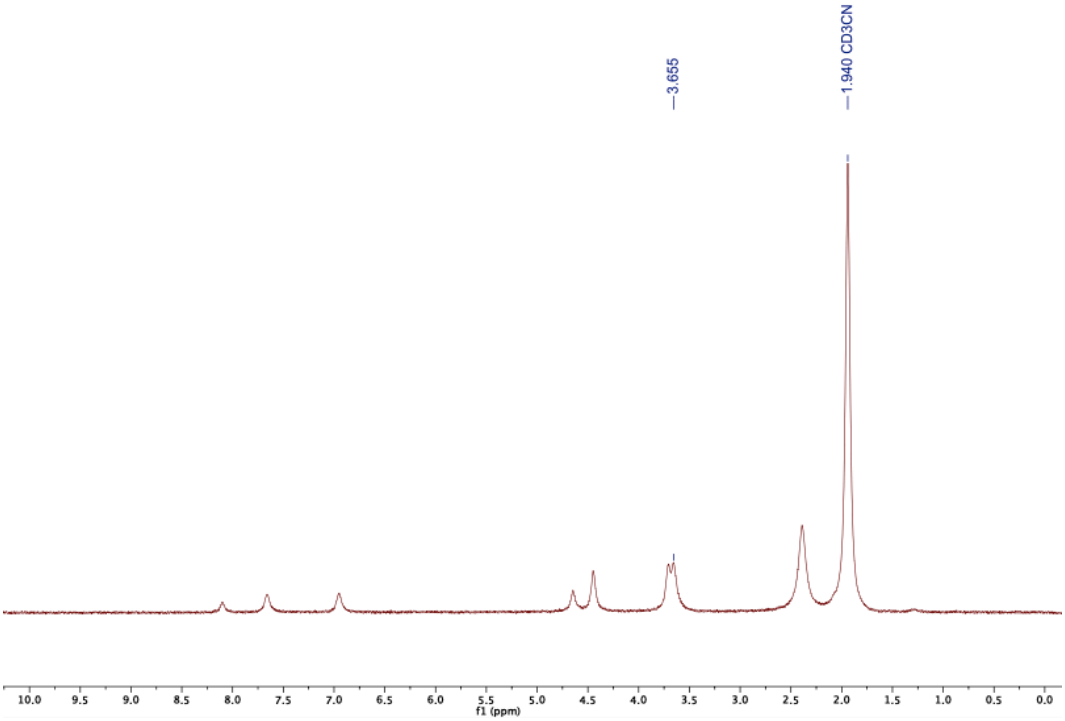

Figure S14. ^{1}H-NMR (500 MHz) of compound **7** + 4 equiv. of $NaPF_6$ in CD_3CN.

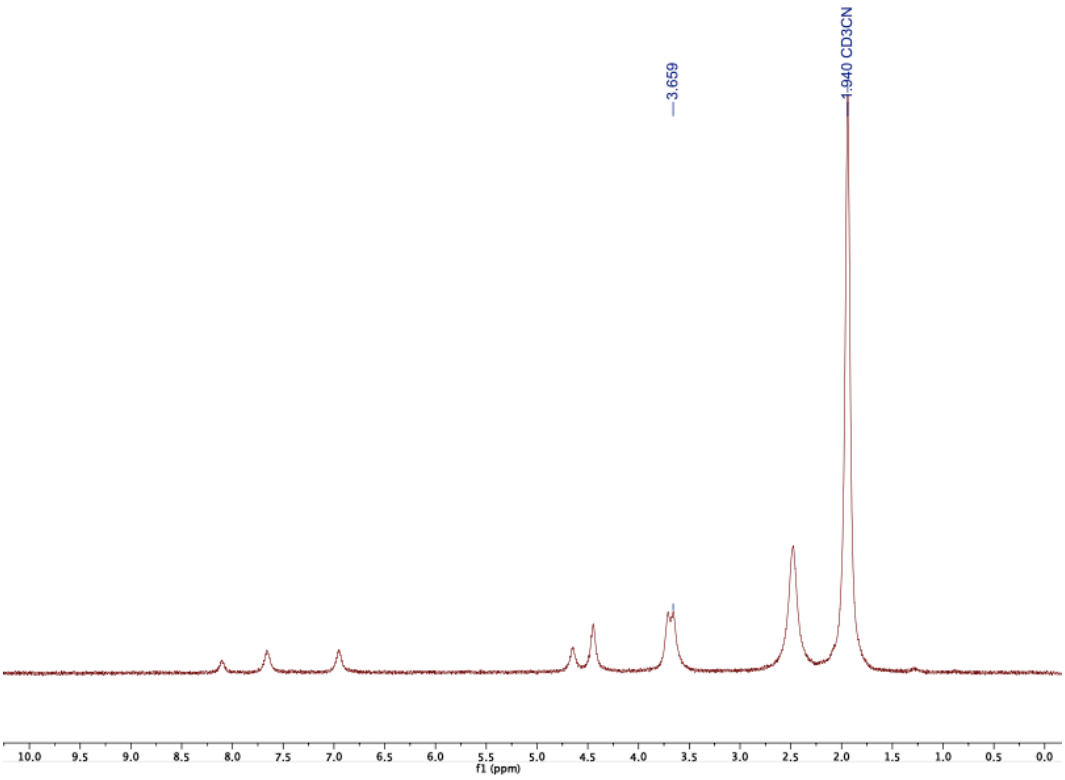

Figure S15. ^{1}H-NMR (500 MHz) of compound **7** + 6 equiv. of $NaPF_6$ in CD_3CN.

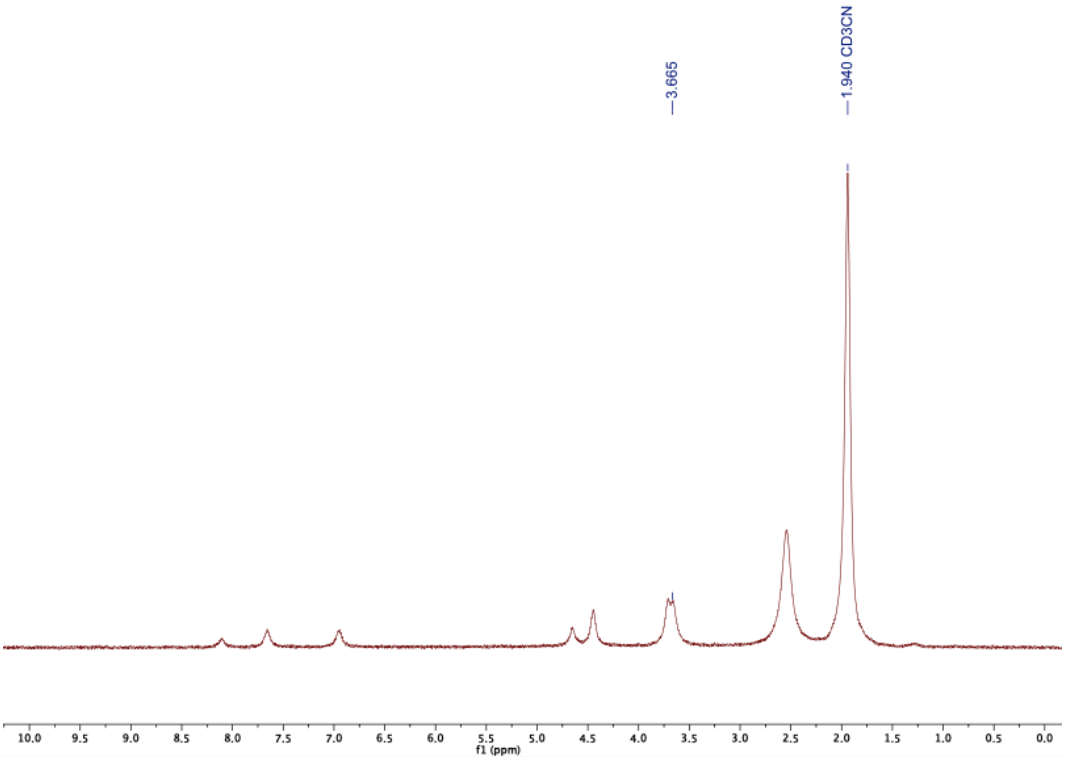

Figure S16. ^{1}H-NMR (500 MHz) of compound **7** + 8 equiv. of $NaPF_6$ in CD_3CN.

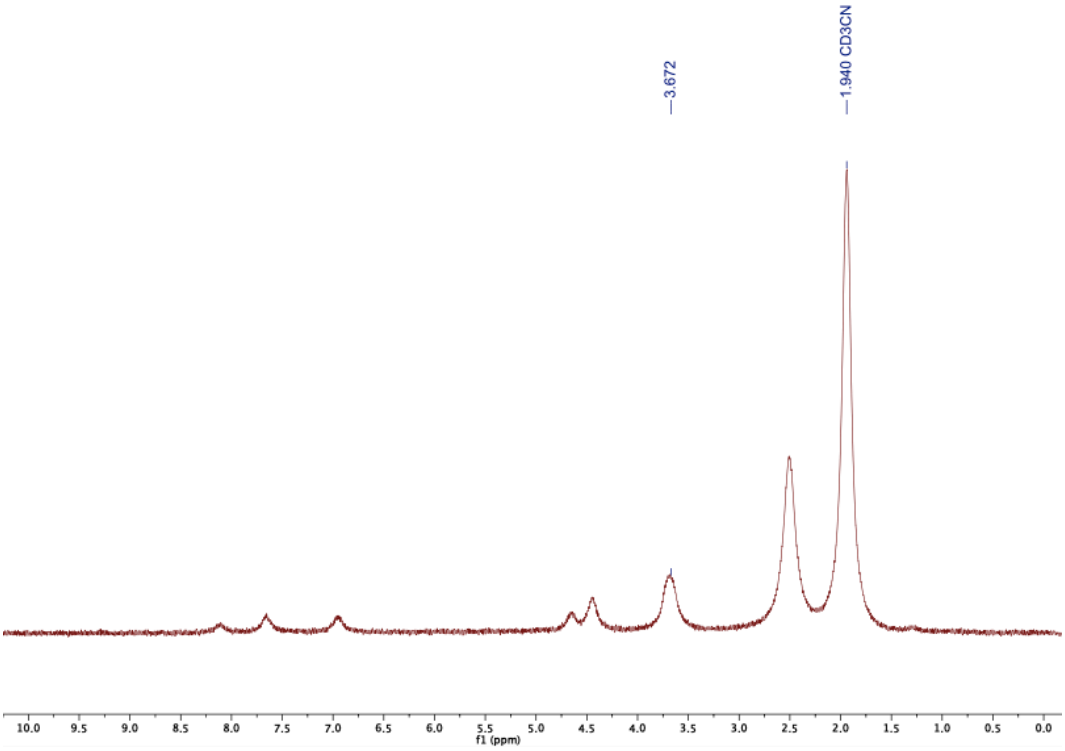

Figure S17. ^{1}H-NMR (500 MHz) of compound **7** + 10 equiv. of $NaPF_6$ in CD_3CN.

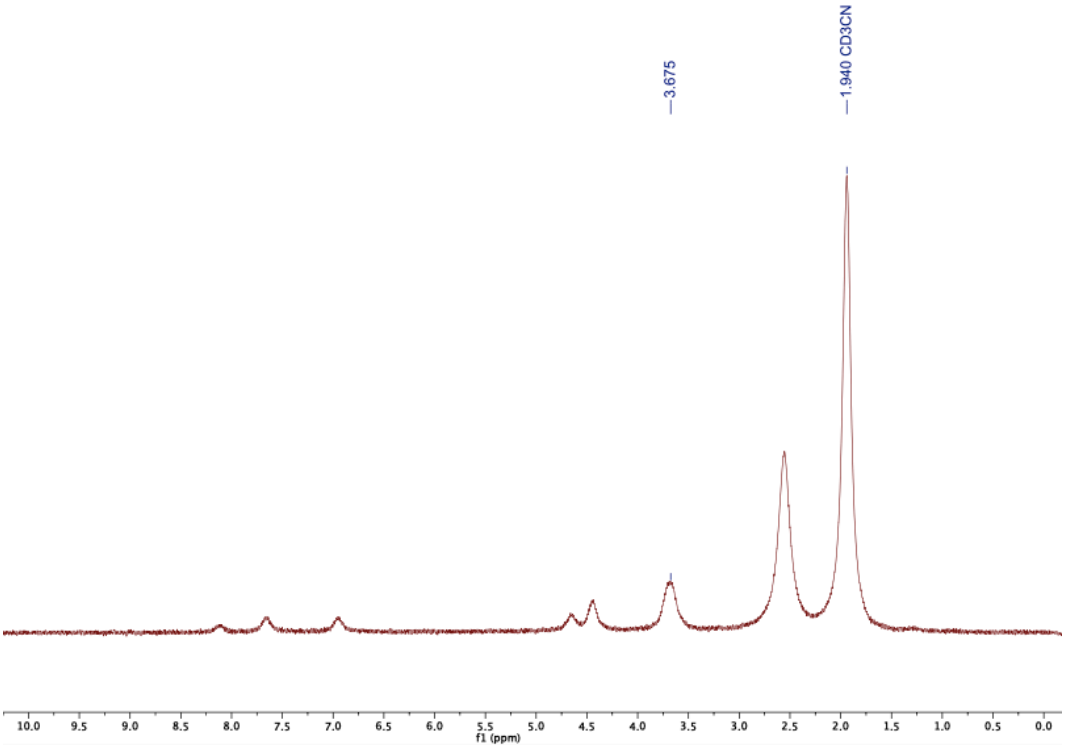

Figure S18. ^{1}H-NMR (500 MHz) of compound **7** + 12 equiv. of $NaPF_6$ in CD_3CN.

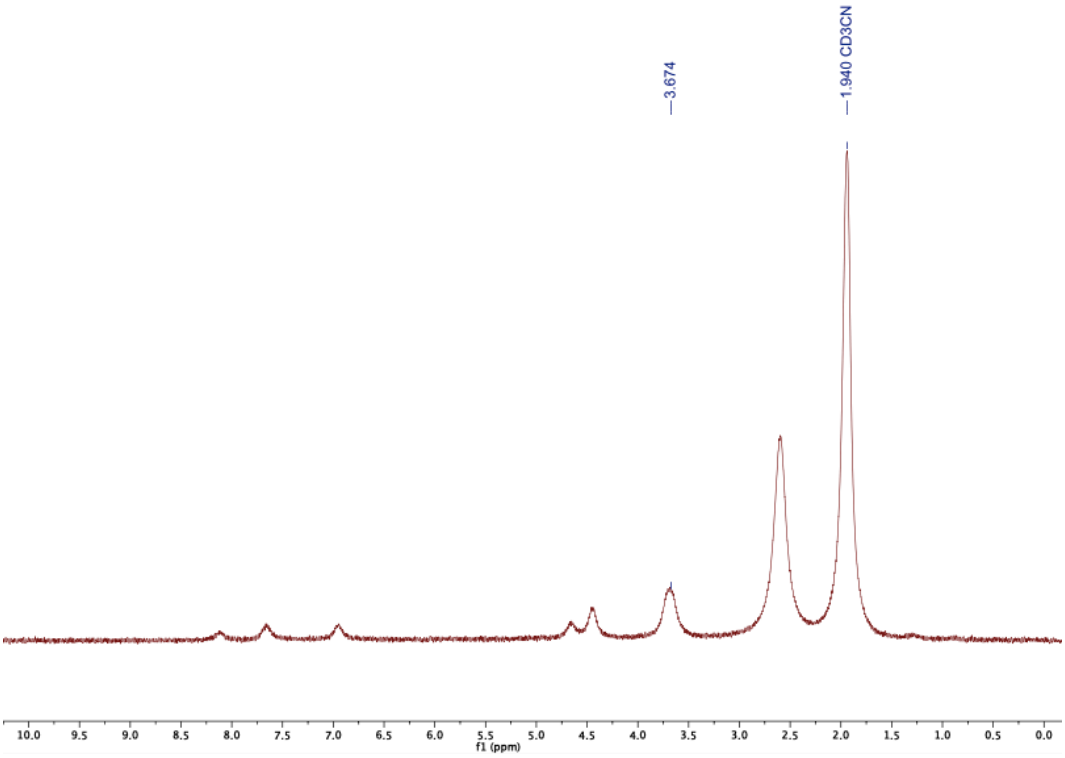

Figure S19. ^{1}H-NMR (500 MHz) of compound **7** + 14 equiv. of $NaPF_6$ in CD_3CN.

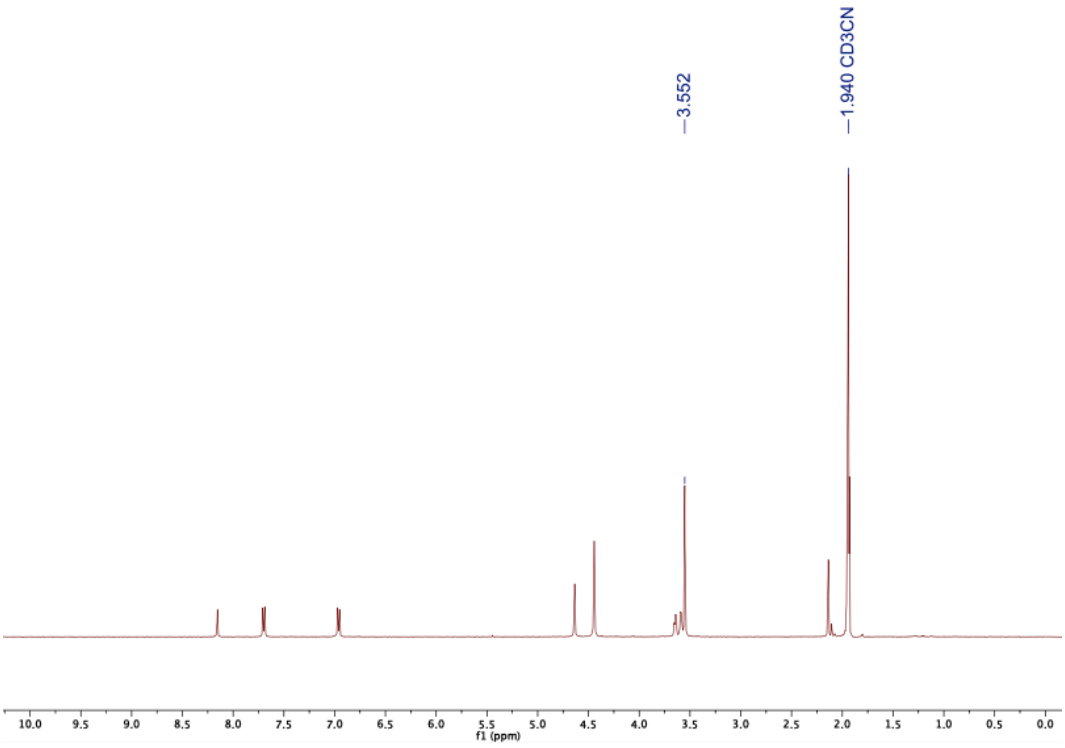

Figure S20. ^{1}H-NMR (500 MHz) of compound **7** + 0 equiv. of KPF_6 in CD_3CN.

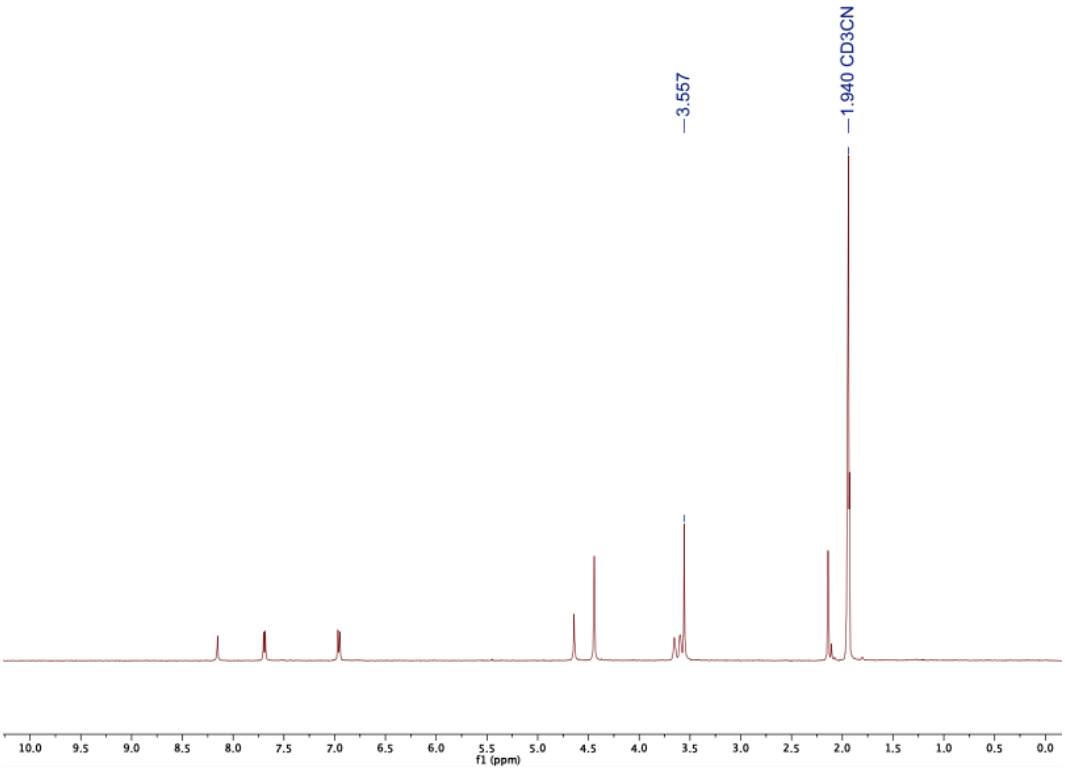

Figure S21. ^{1}H-NMR (500 MHz) of compound **7** + 0.1 equiv. of KPF_6 in CD_3CN.

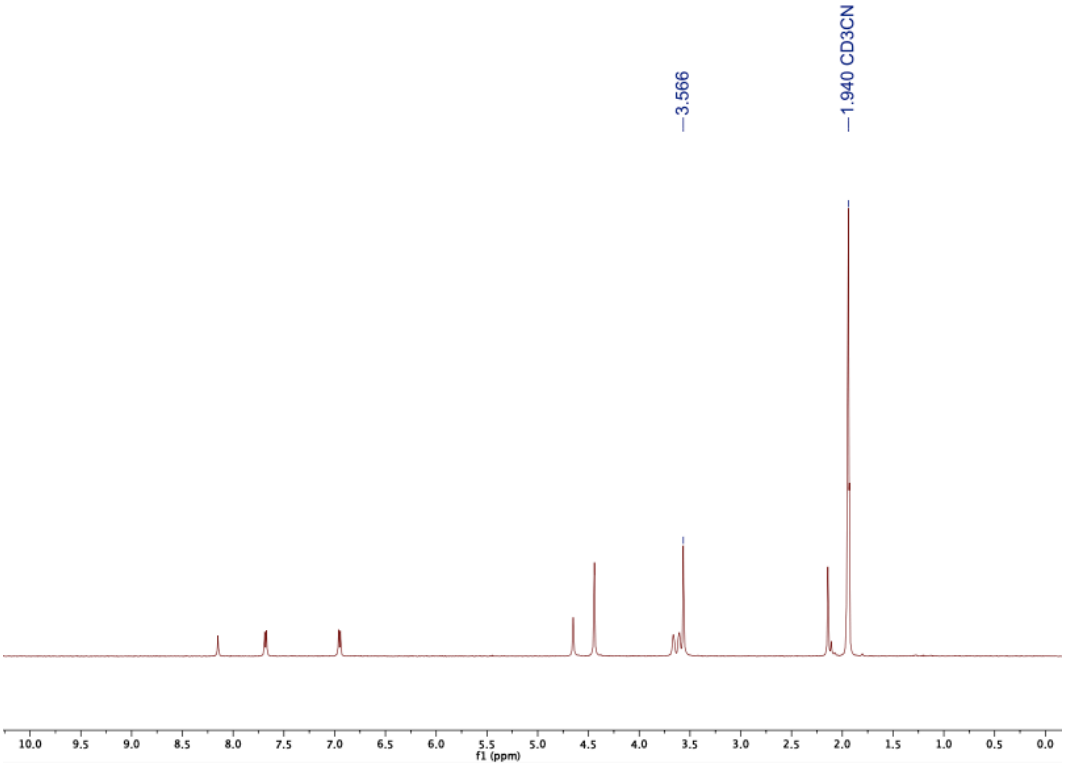

Figure S22. ^{1}H-NMR (500 MHz) of compound **7** + 0.3 equiv. of KPF_6 in CD_3CN.

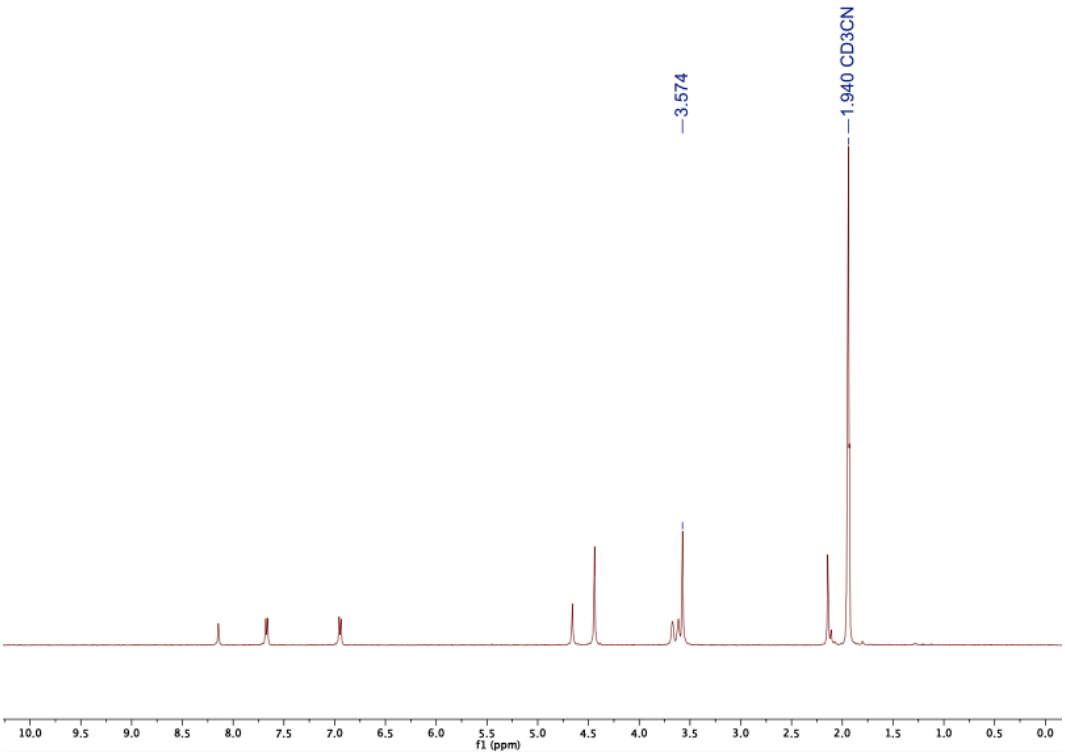

Figure S23. ^{1}H-NMR (500 MHz) of compound **7** + 0.5 equiv. of KPF_6 in CD_3CN.

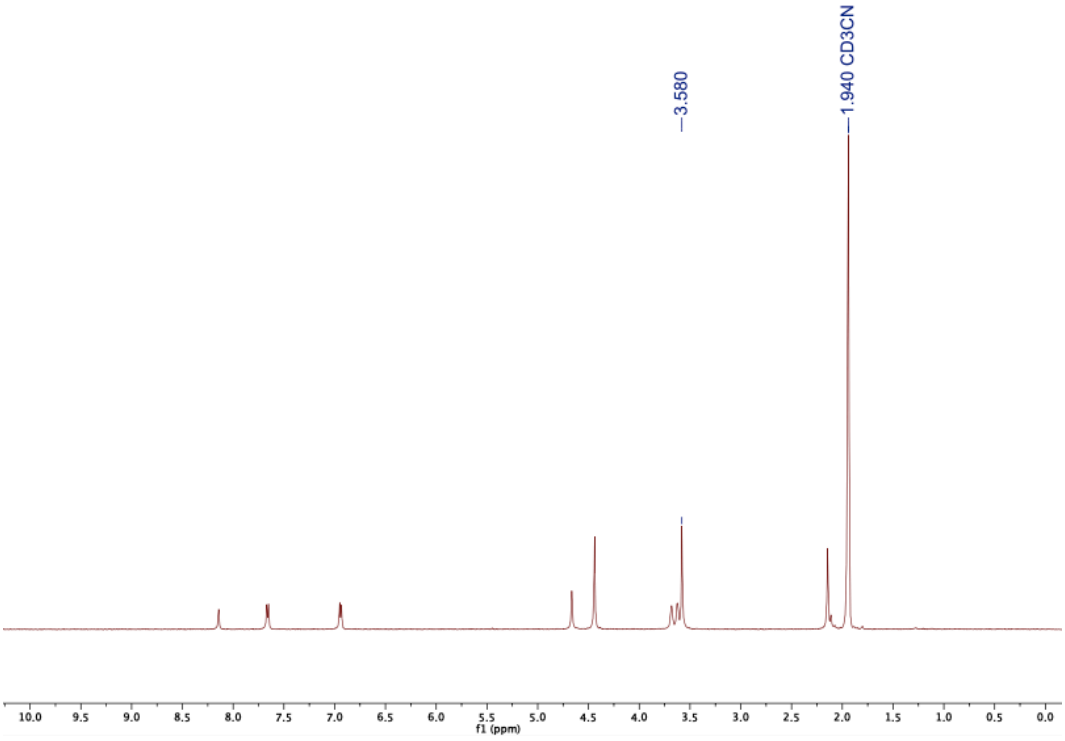

Figure S24. ^{1}H-NMR (500 MHz) of compound **7** + 0.7 equiv. of KPF_6 in CD_3CN.

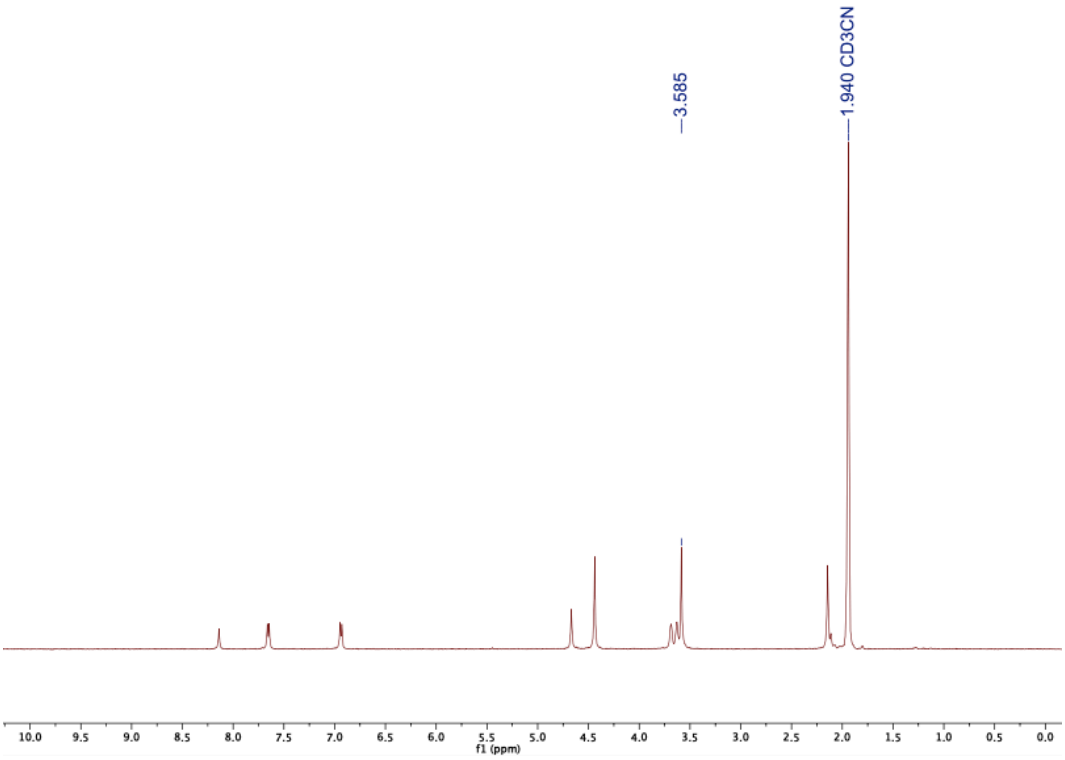

Figure S25. ^{1}H-NMR (500 MHz) of compound **7** + 0.9 equiv. of KPF_6 in CD_3CN.

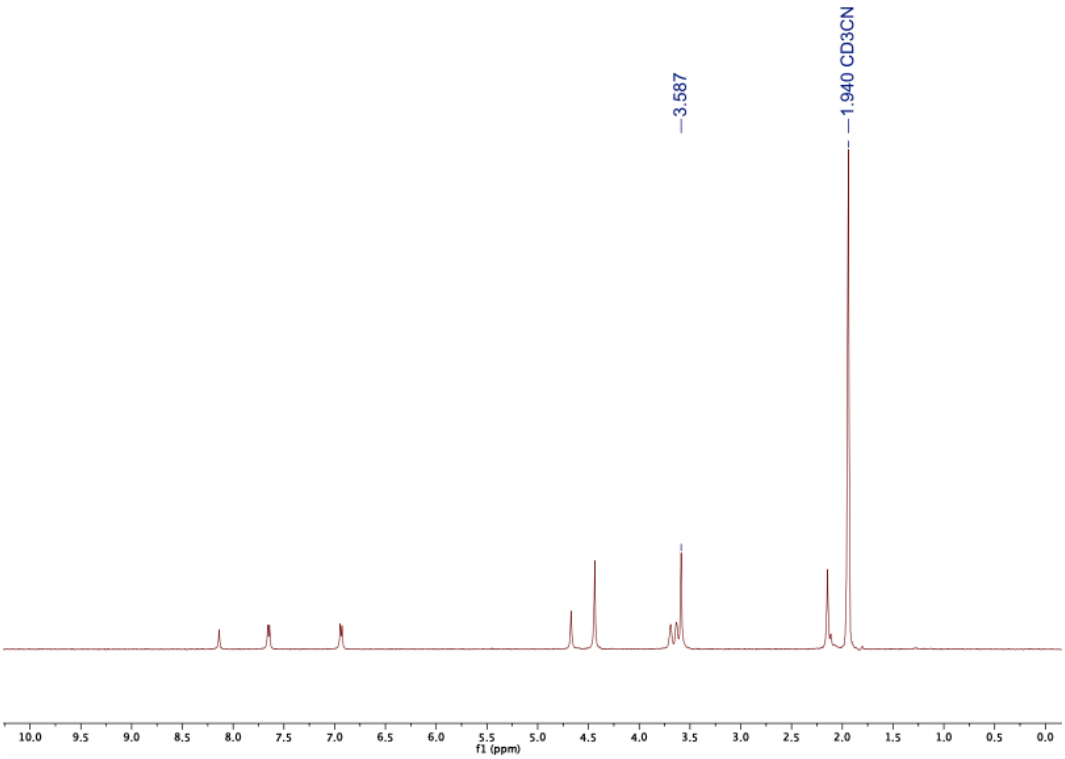

Figure S26. ^{1}H-NMR (500 MHz) of compound **7** + 1 equiv. of KPF_6 in CD_3CN.

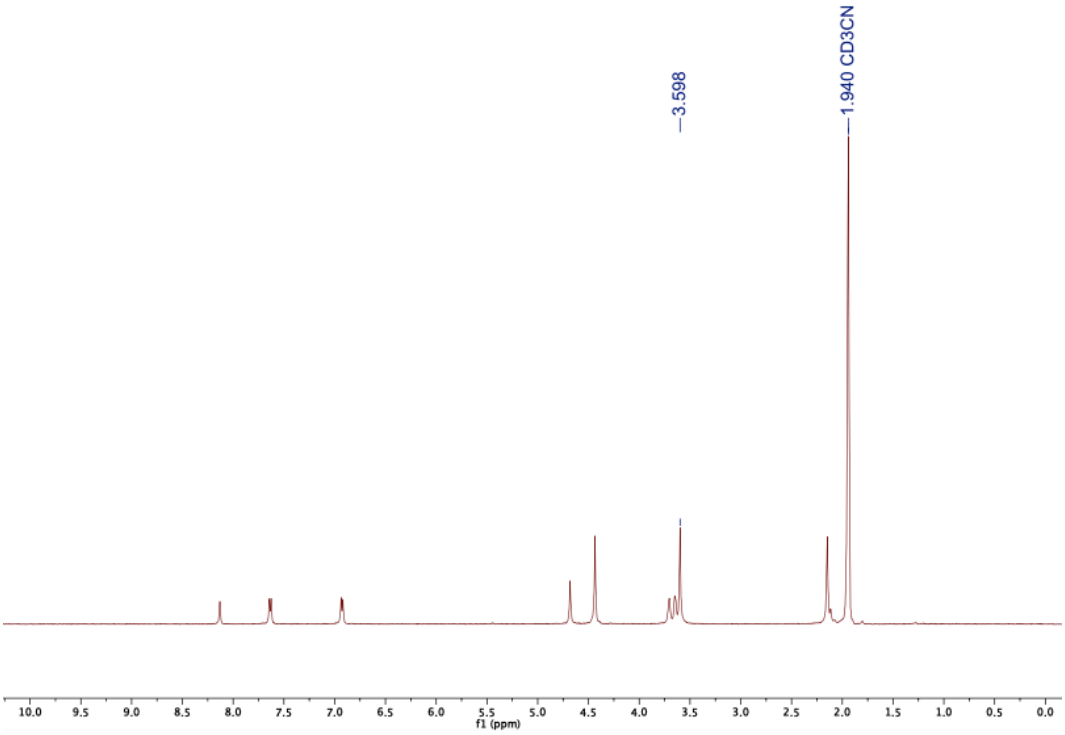

Figure S27. ^{1}H-NMR (500 MHz) of compound **7** + 2 equiv. of KPF_6 in CD_3CN.

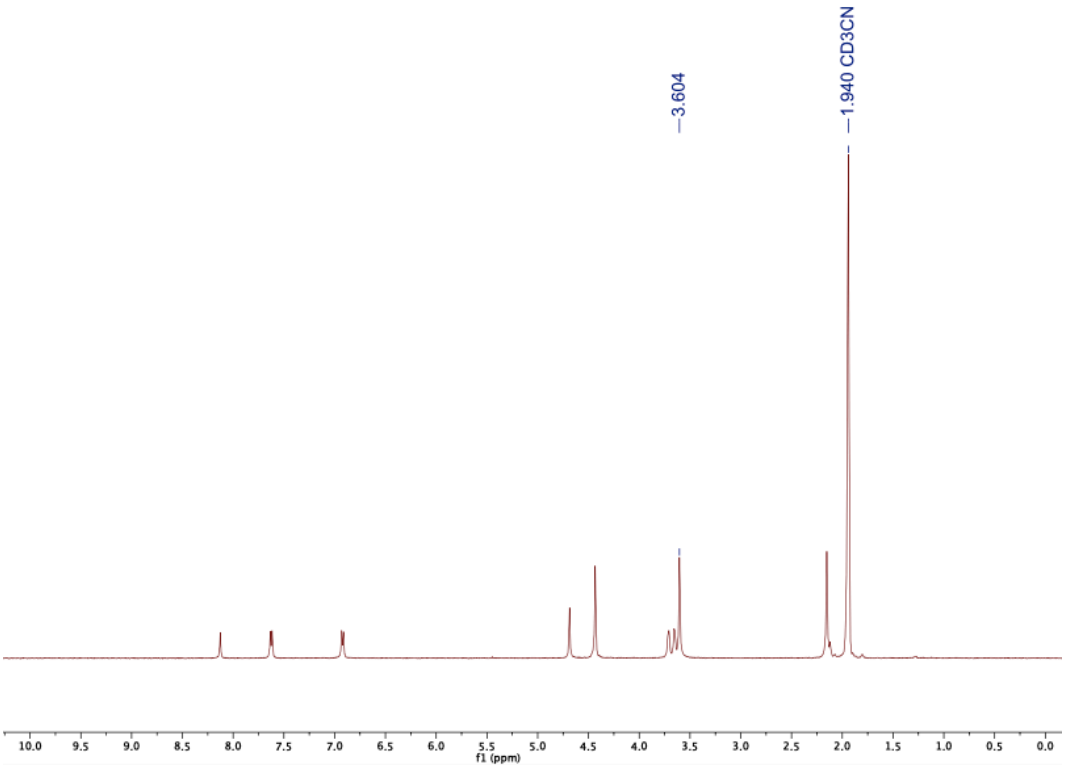

Figure S28. ^{1}H-NMR (500 MHz) of compound **7** + 4 equiv. of KPF_6 in CD_3CN.

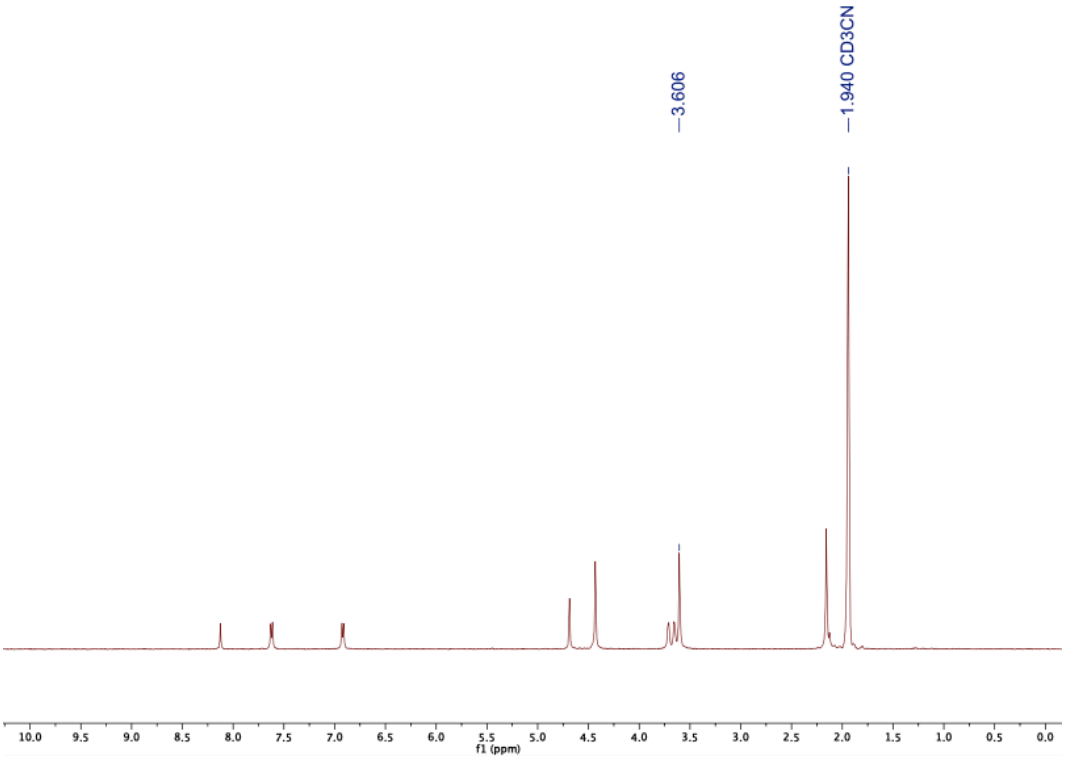

Figure S29. ^{1}H-NMR (500 MHz) of compound **7** + 6 equiv. of KPF_6 in CD_3CN.

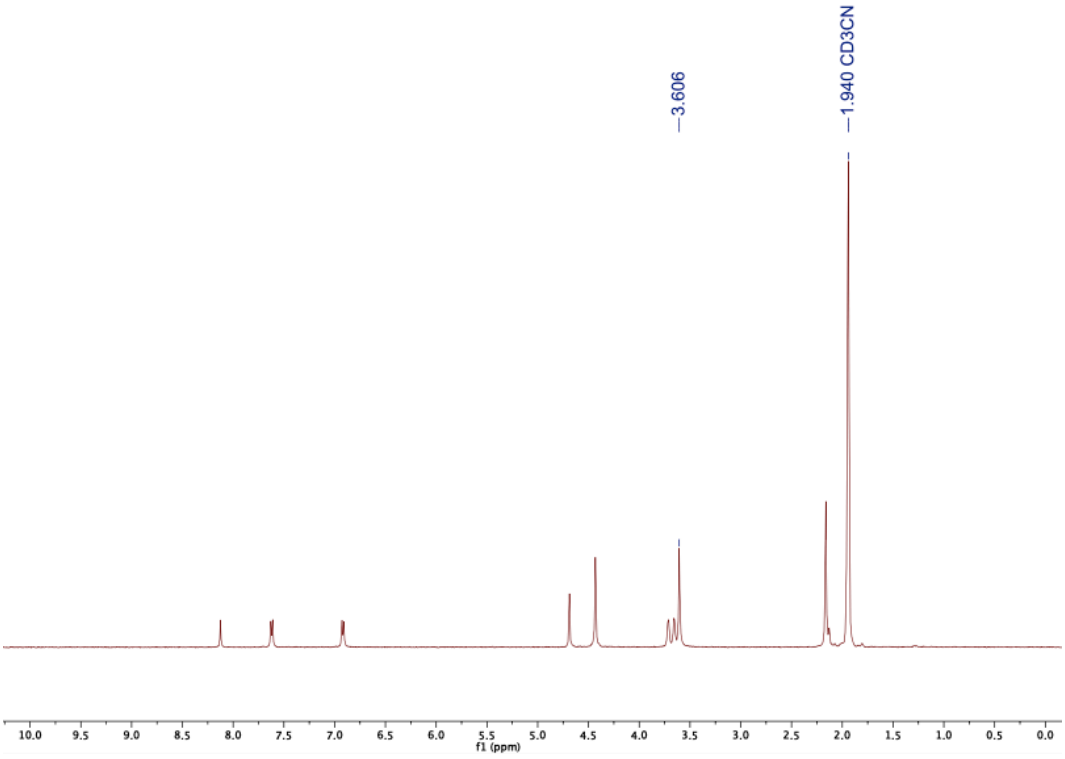

Figure S30. ^{1}H-NMR (500 MHz) of compound **7** + 8 equiv. of KPF_6 in CD_3CN.

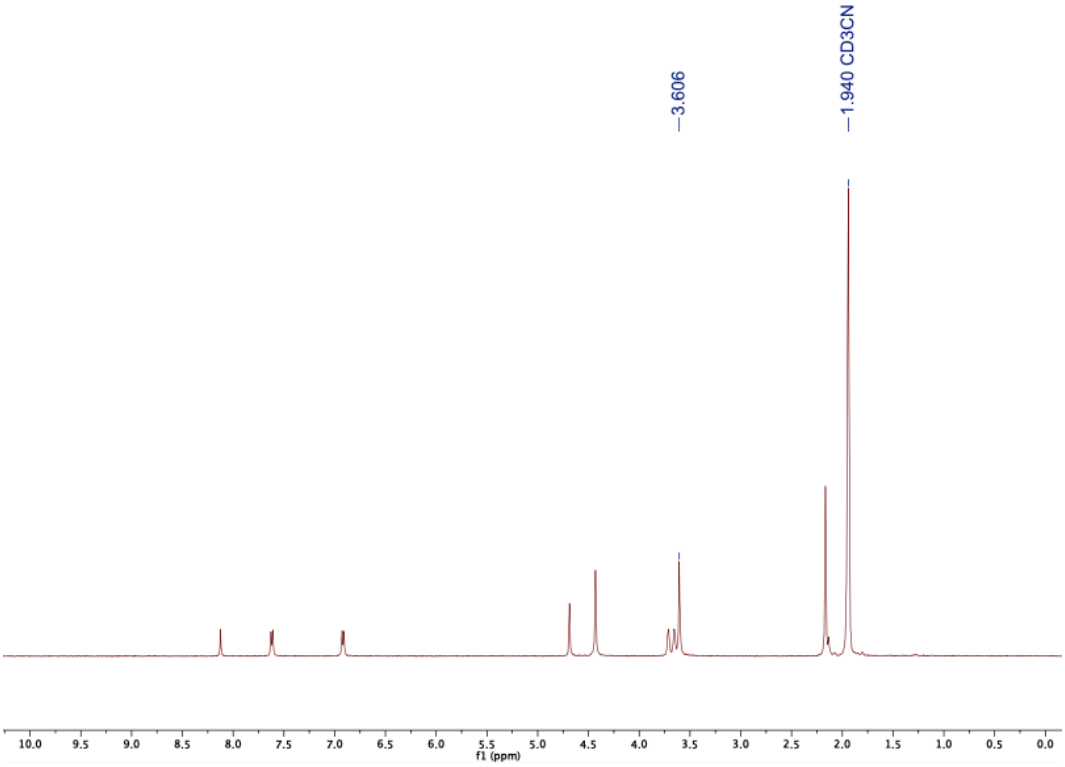

Figure S31. ^{1}H-NMR (500 MHz) of compound **7** + 10 equiv. of KPF_6 in CD_3CN.

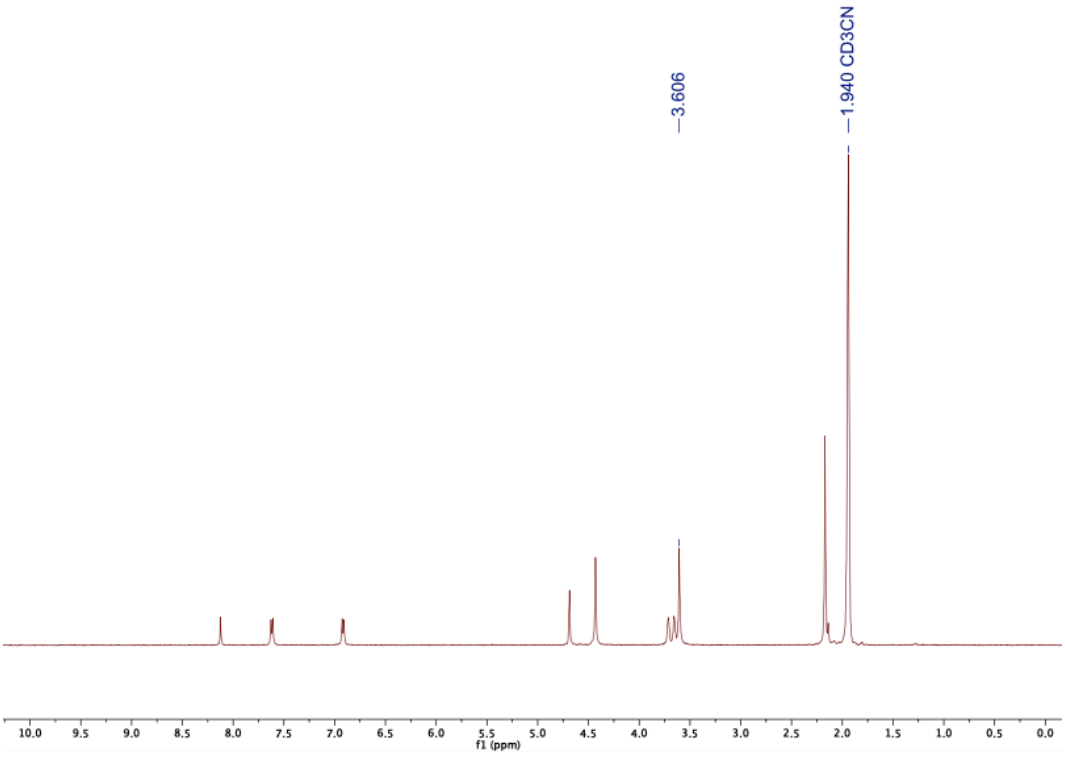

Figure S32. ^{1}H-NMR (500 MHz) of compound **7** + 12 equiv. of KPF_6 in CD_3CN.

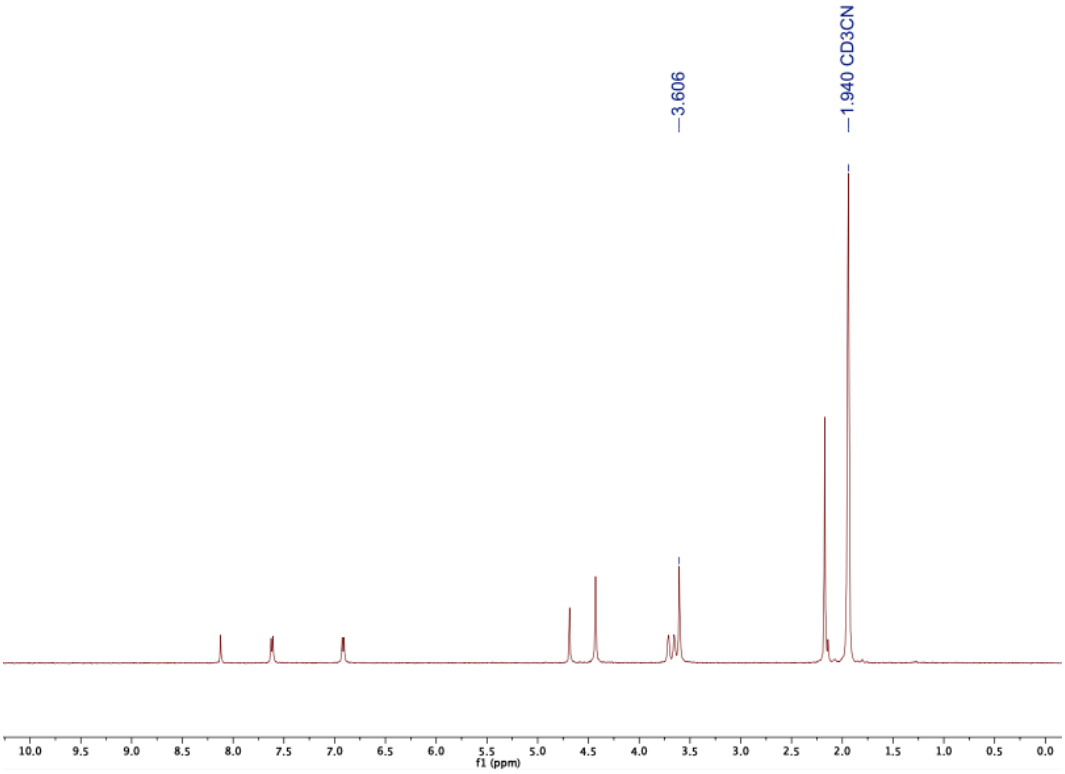

Figure S33. ^{1}H-NMR (500 MHz) of compound **7** + 14 equiv. of KPF_6 in CD_3CN.

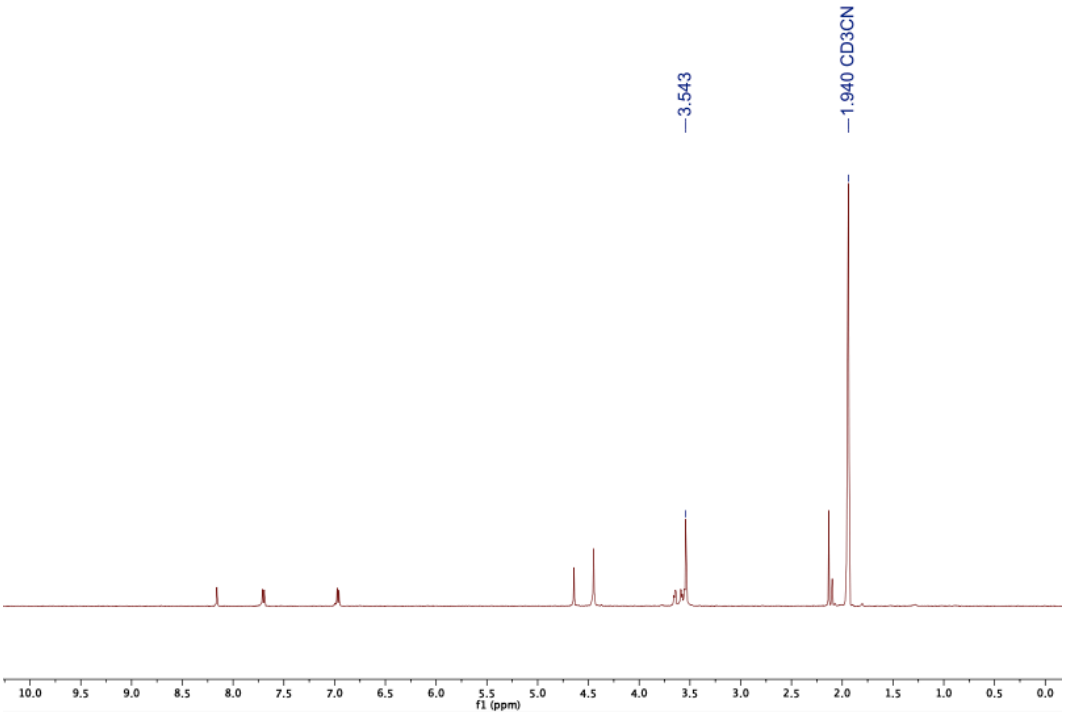

Figure S34. ^{1}H-NMR (500 MHz) of compound **8** + 0 equiv. of $NaPF_6$ in CD_3CN.

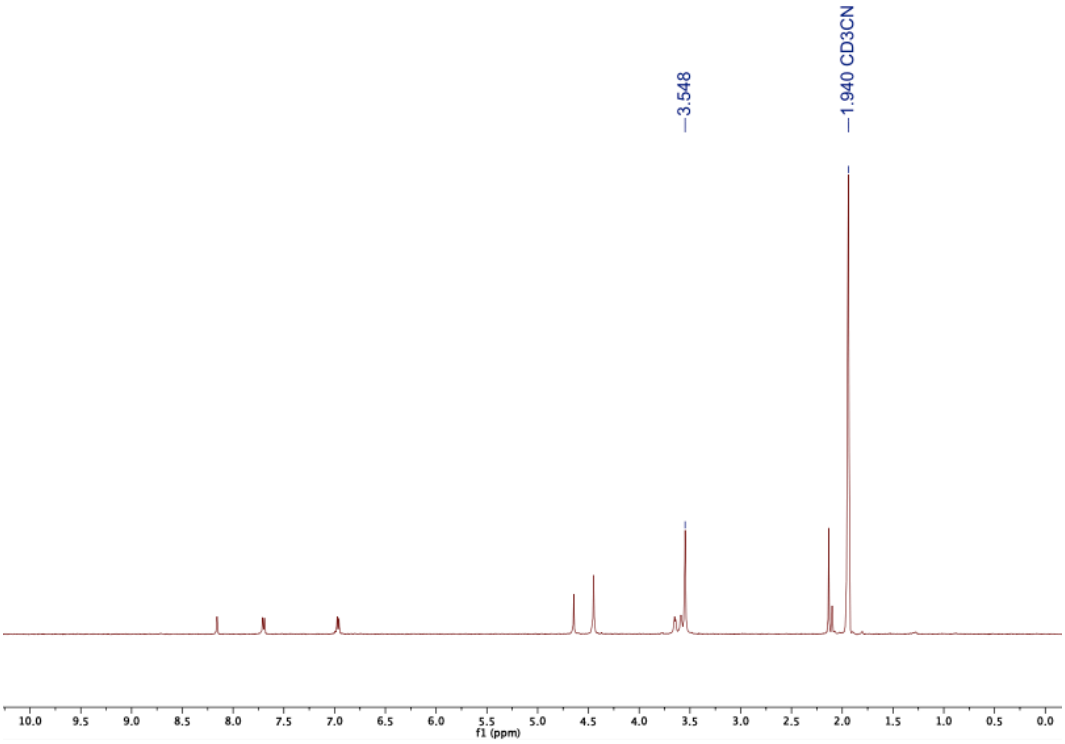

Figure S35. ^{1}H-NMR (500 MHz) of compound **8** + 0.1 equiv. of $NaPF_6$ in CD_3CN.

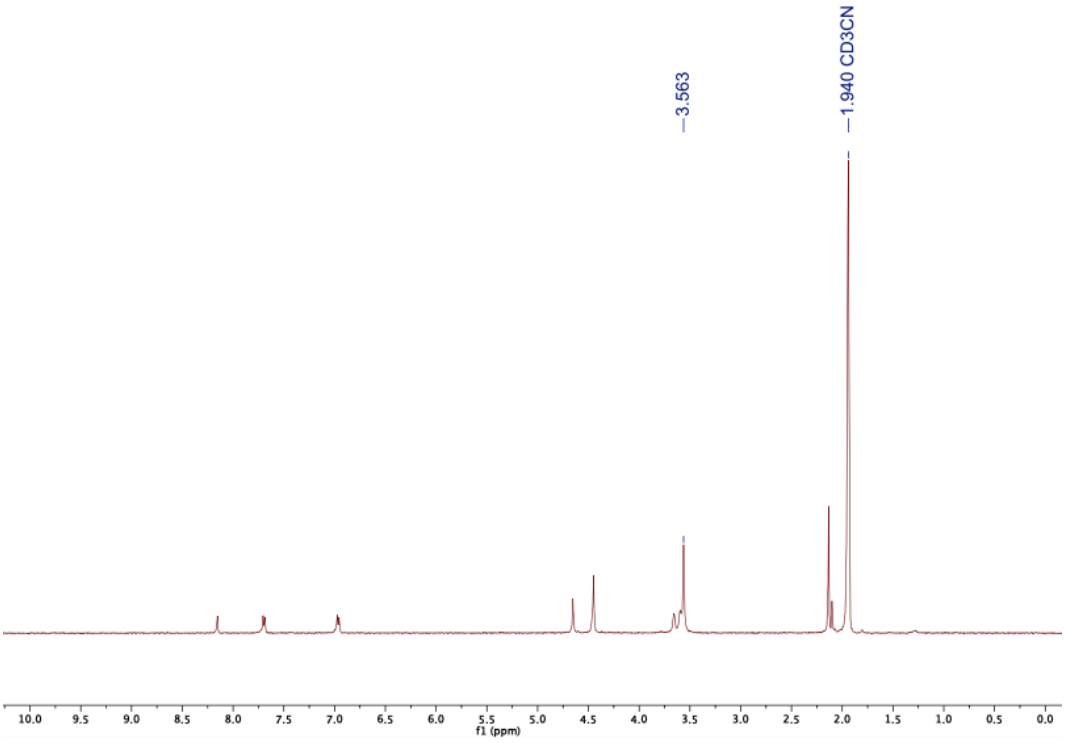

Figure S36. ^{1}H-NMR (500 MHz) of compound **8** + 0.3 equiv. of $NaPF_6$ in CD_3CN.

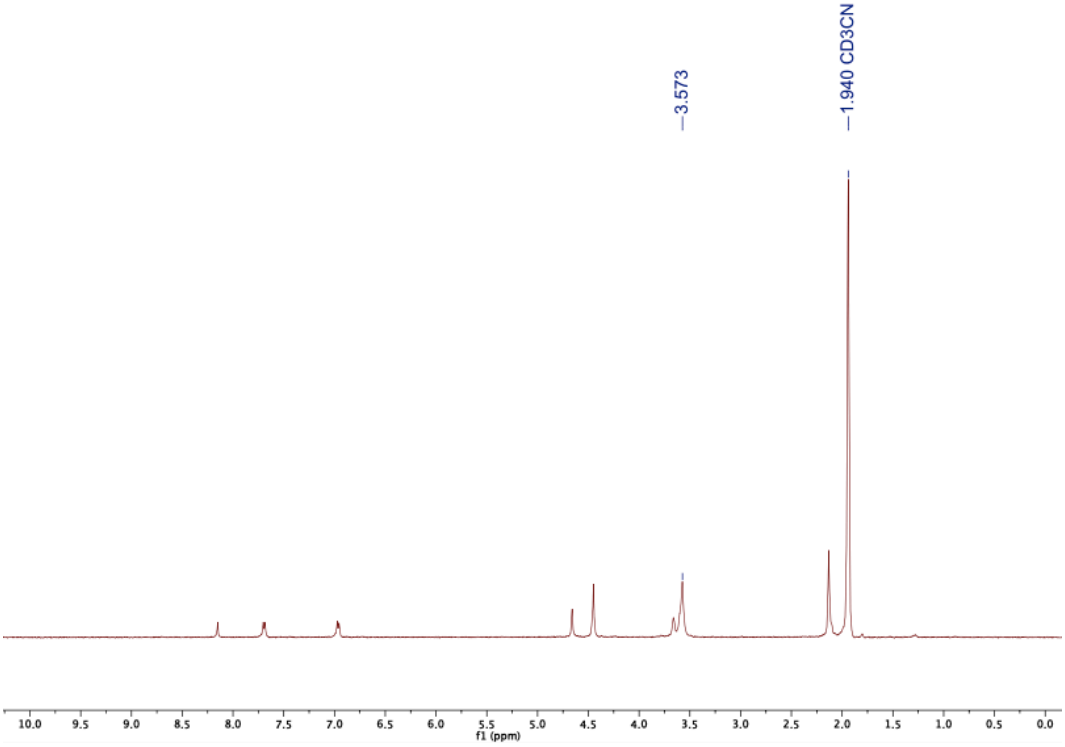

Figure S37. ^{1}H-NMR (500 MHz) of compound **8** + 0.5 equiv. of $NaPF_6$ in CD_3CN.

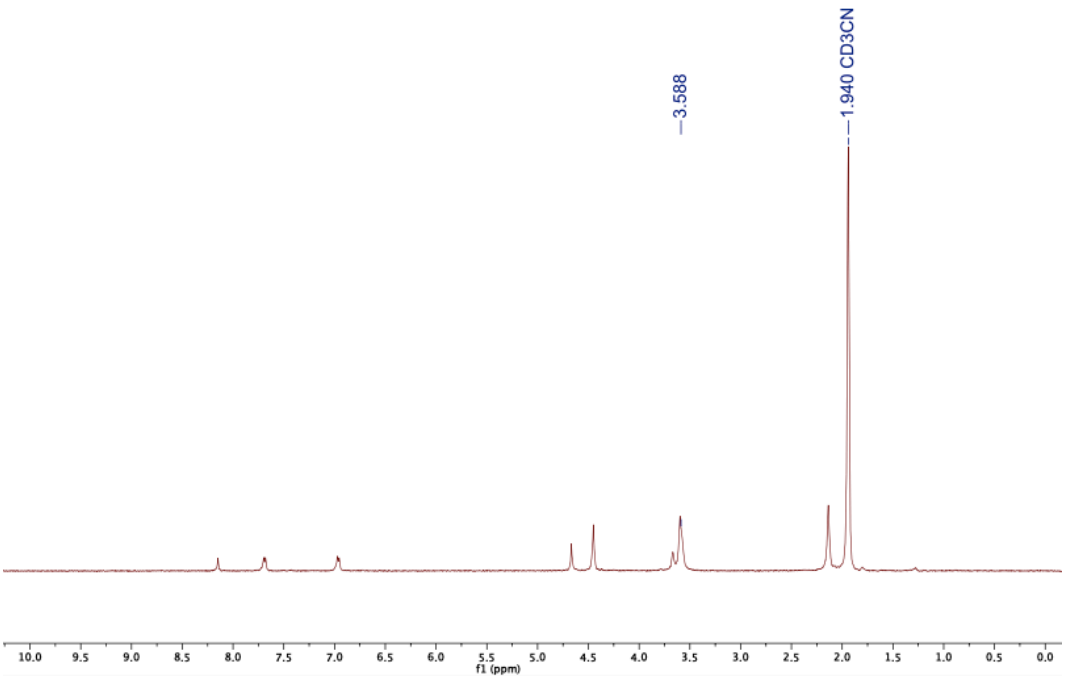

Figure S38. ^{1}H-NMR (500 MHz) of compound **8** + 0.7 equiv. of $NaPF_6$ in CD_3CN.

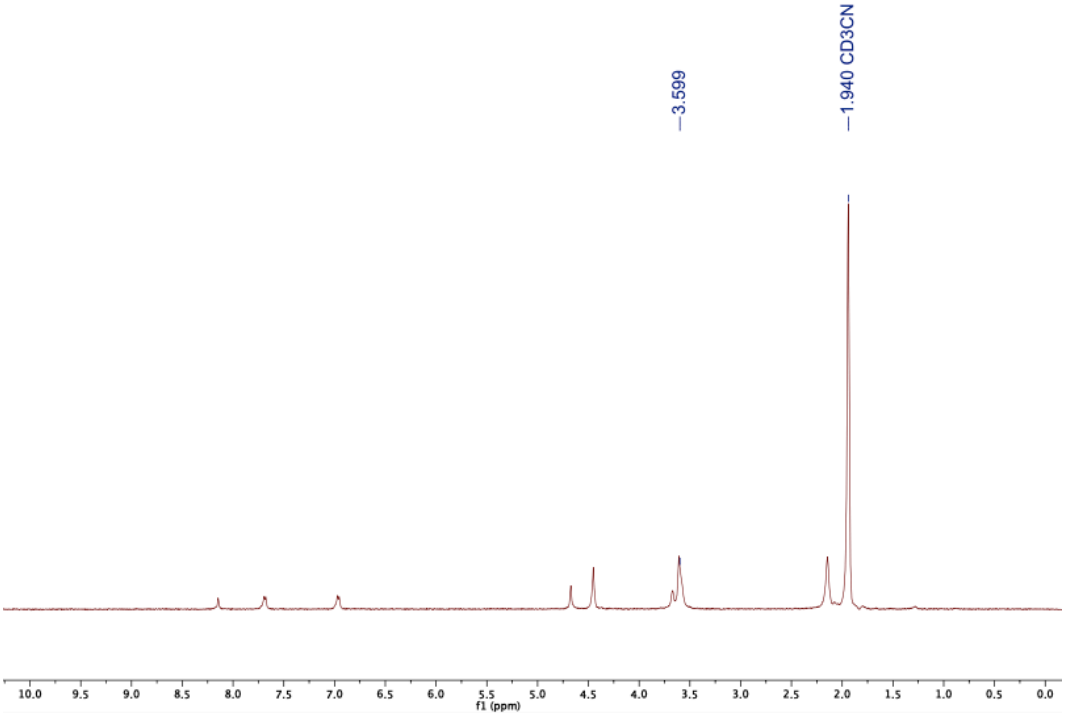

Figure S39. ^{1}H-NMR (500 MHz) of compound **8** + 0.9 equiv. of $NaPF_6$ in CD_3CN.

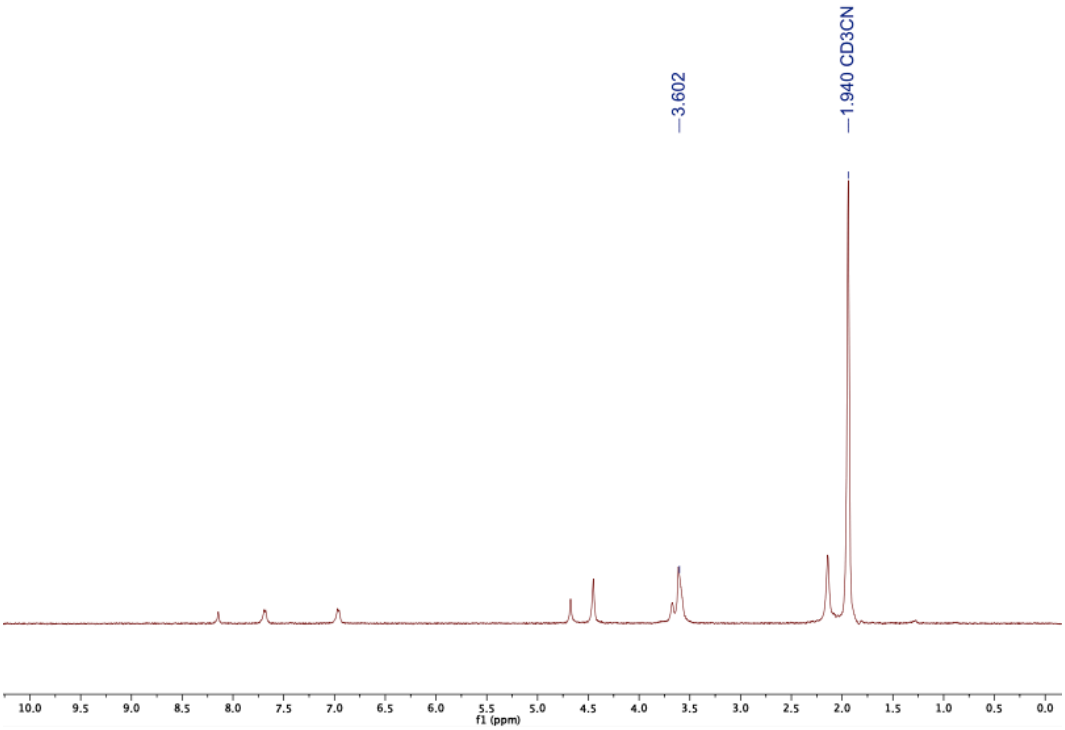

Figure S40. ^{1}H-NMR (500 MHz) of compound **8** + 1 equiv. of $NaPF_6$ in CD_3CN.

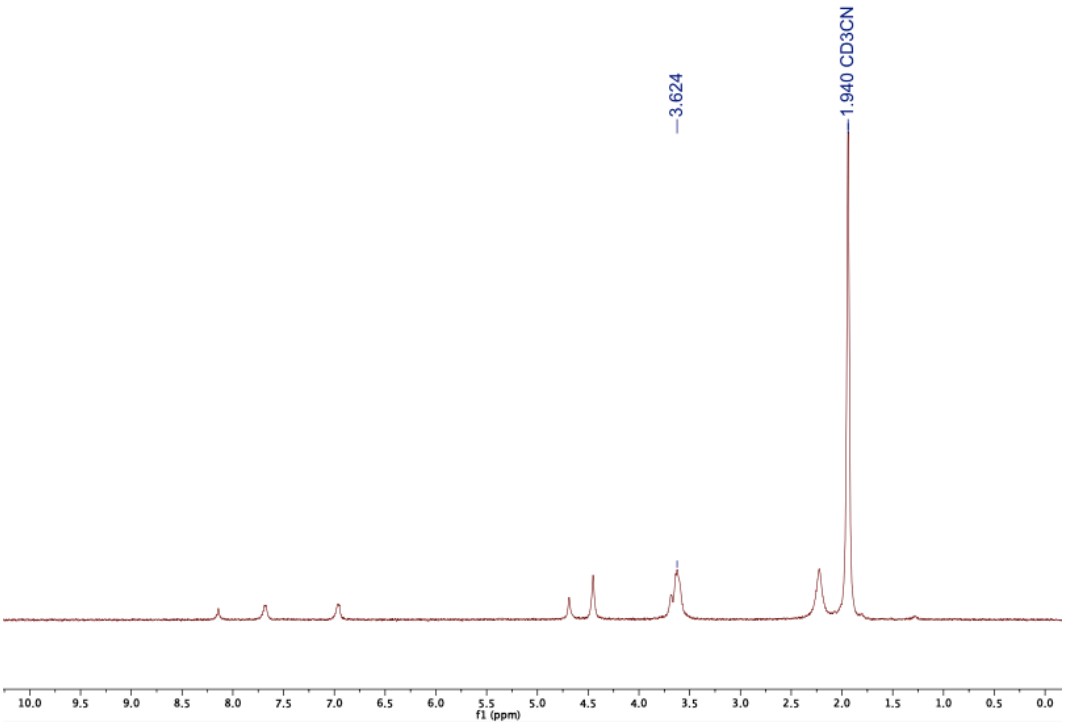

Figure S41. ^{1}H-NMR (500 MHz) of compound **8** + 2 equiv. of $NaPF_6$ in CD_3CN.

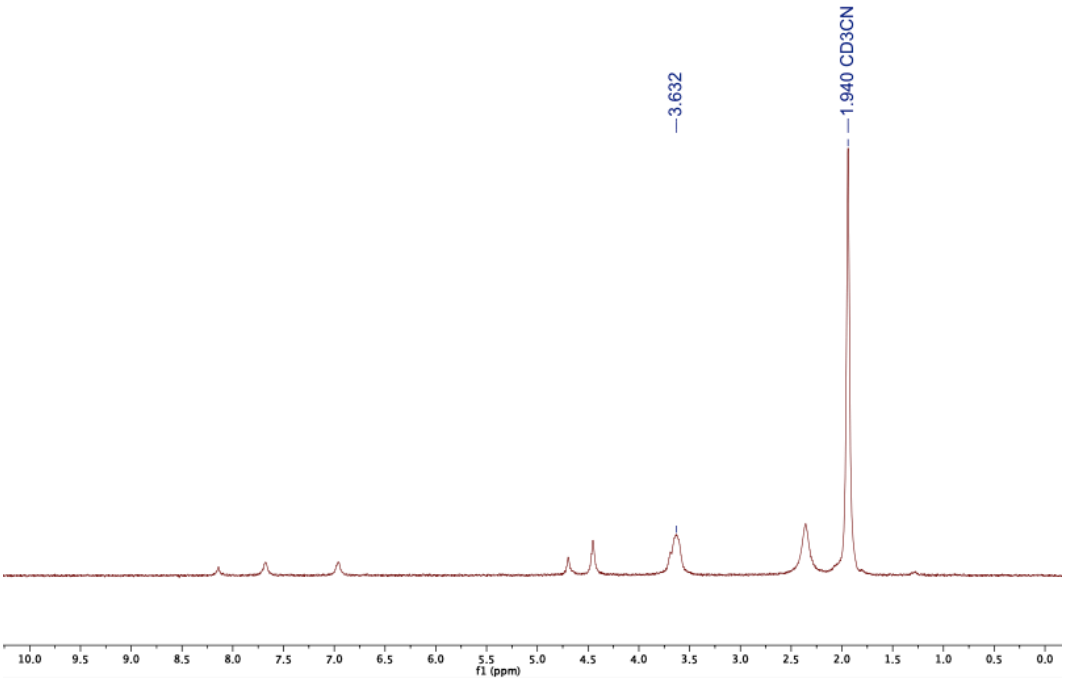

Figure S42. ^{1}H-NMR (500 MHz) of compound **8** + 4 equiv. of $NaPF_6$ in CD_3CN.

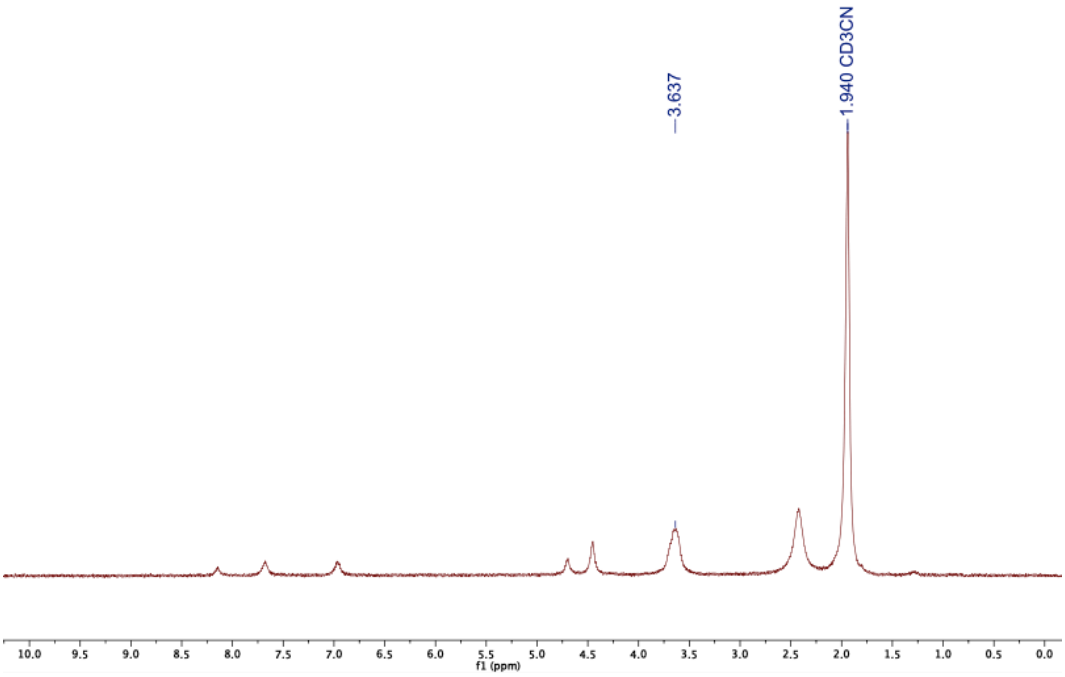

Figure S43. ^{1}H-NMR (500 MHz) of compound **8** + 6 equiv. of $NaPF_6$ in CD_3CN.

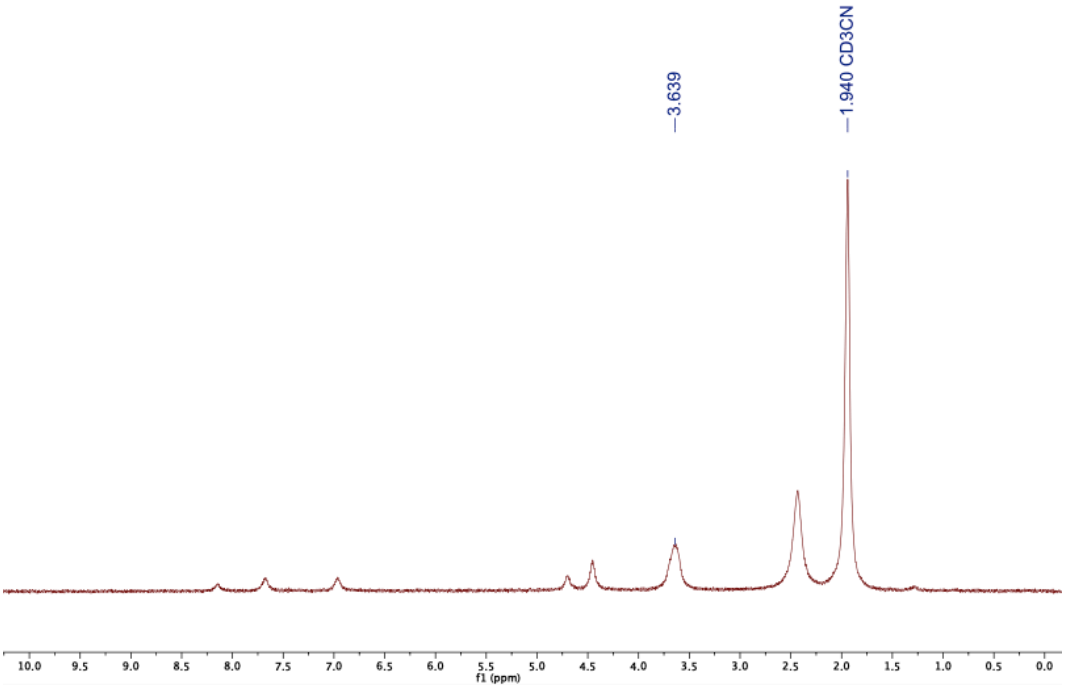

Figure S44. ^{1}H-NMR (500 MHz) of compound **8** + 8 equiv. of $NaPF_6$ in CD_3CN.

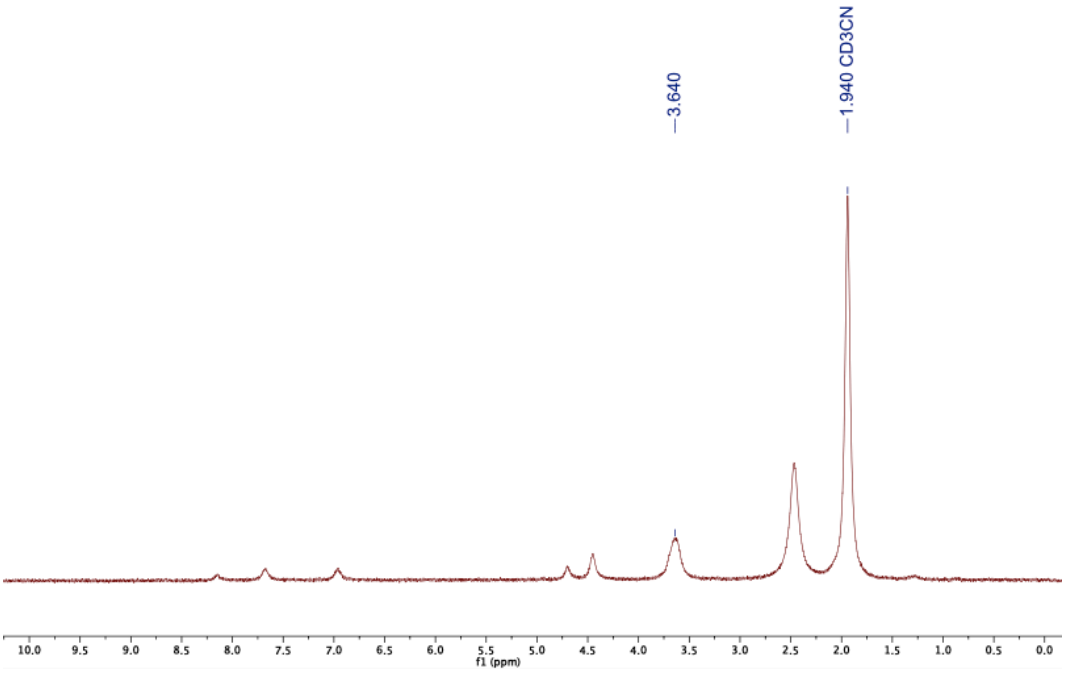

Figure S45. ^{1}H-NMR (500 MHz) of compound **8** + 10 equiv. of $NaPF_6$ in CD_3CN.

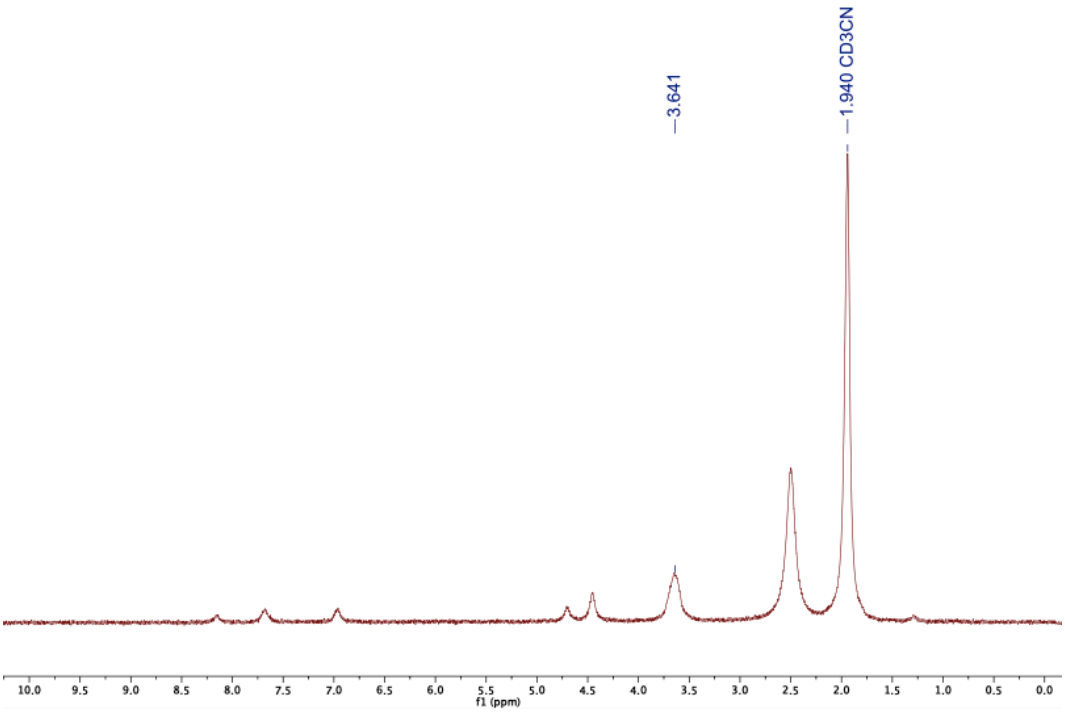

Figure S46. ^{1}H-NMR (500 MHz) of compound **8** + 12 equiv. of $NaPF_6$ in CD_3CN.

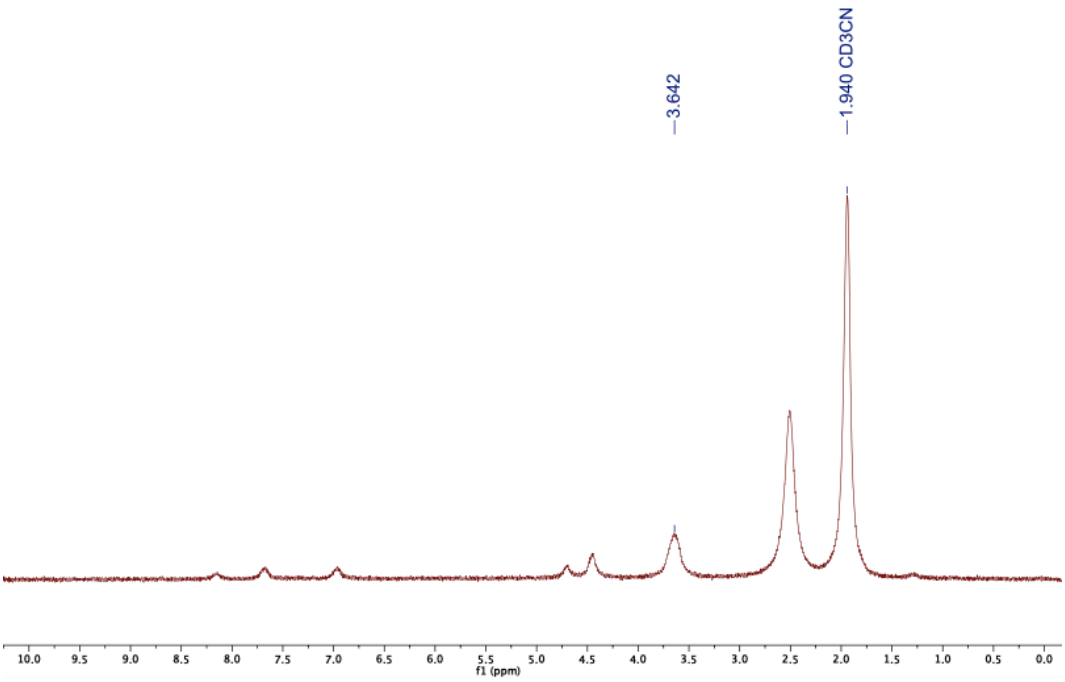

Figure S47. ^{1}H-NMR (500 MHz) of compound **8** + 14 equiv. of $NaPF_6$ in CD_3CN.

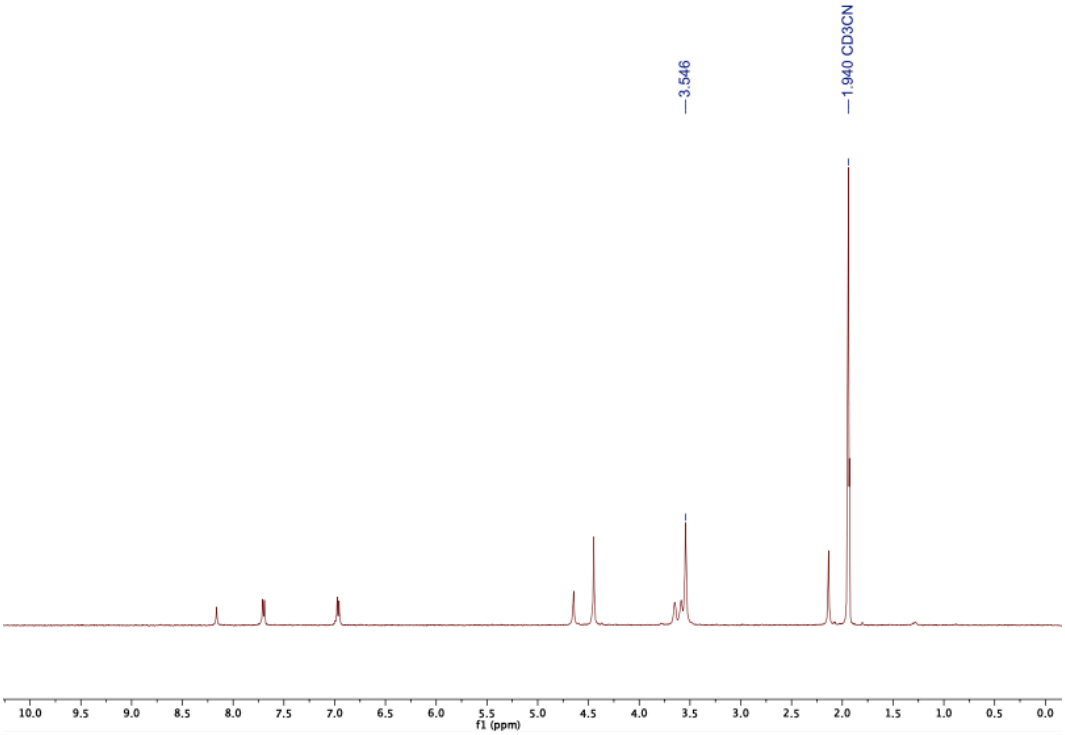

Figure S48. ^{1}H-NMR (500 MHz) of compound **8** + 0 equiv. of KPF_6 in CD_3CN.

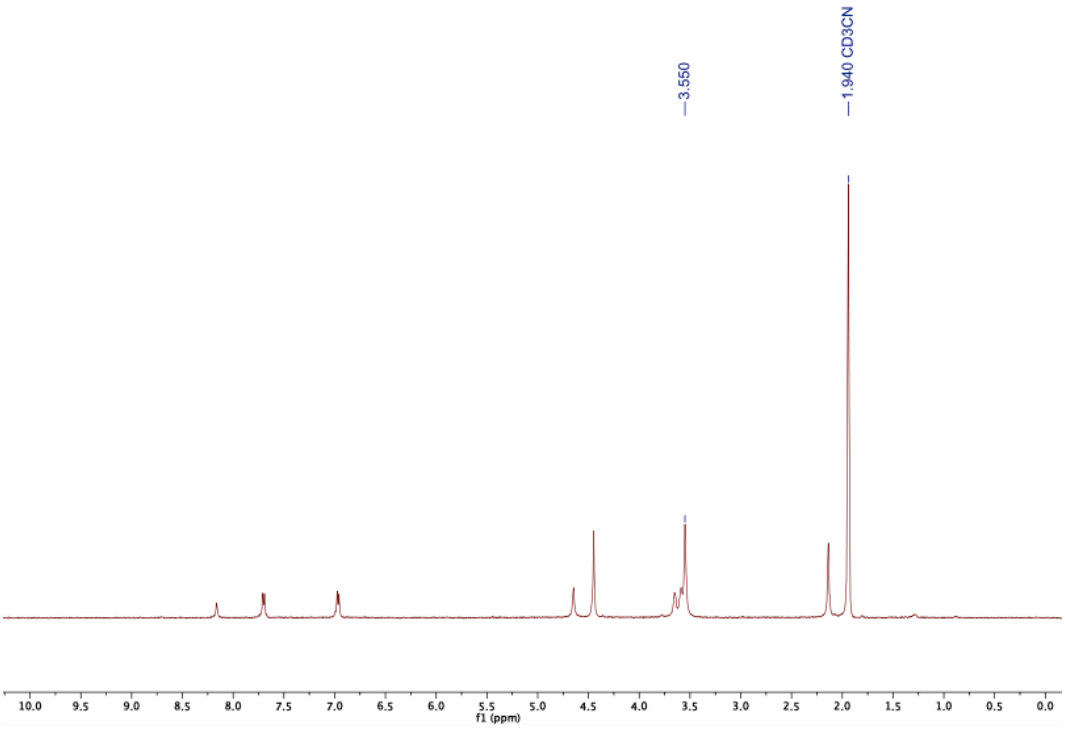

Figure S49. ^{1}H-NMR (500 MHz) of compound **8** + 0.1 equiv. of KPF_6 in CD_3CN.

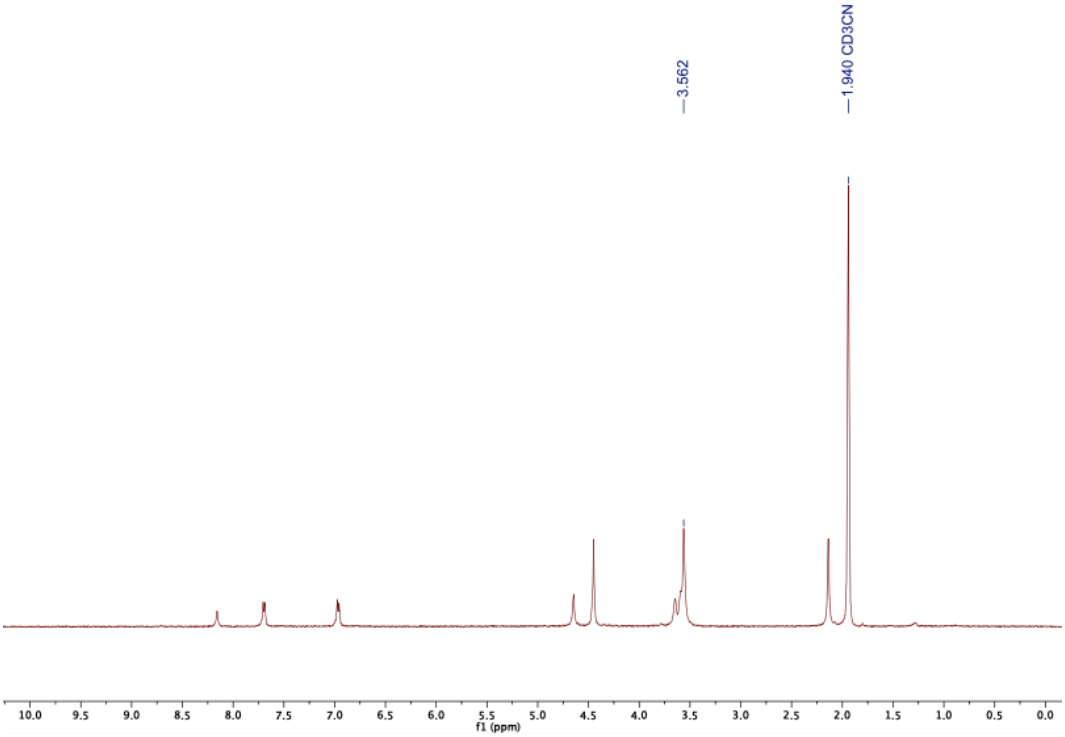

Figure S50. ^{1}H-NMR (500 MHz) of compound **8** + 0.3 equiv. of KPF_6 in CD_3CN.

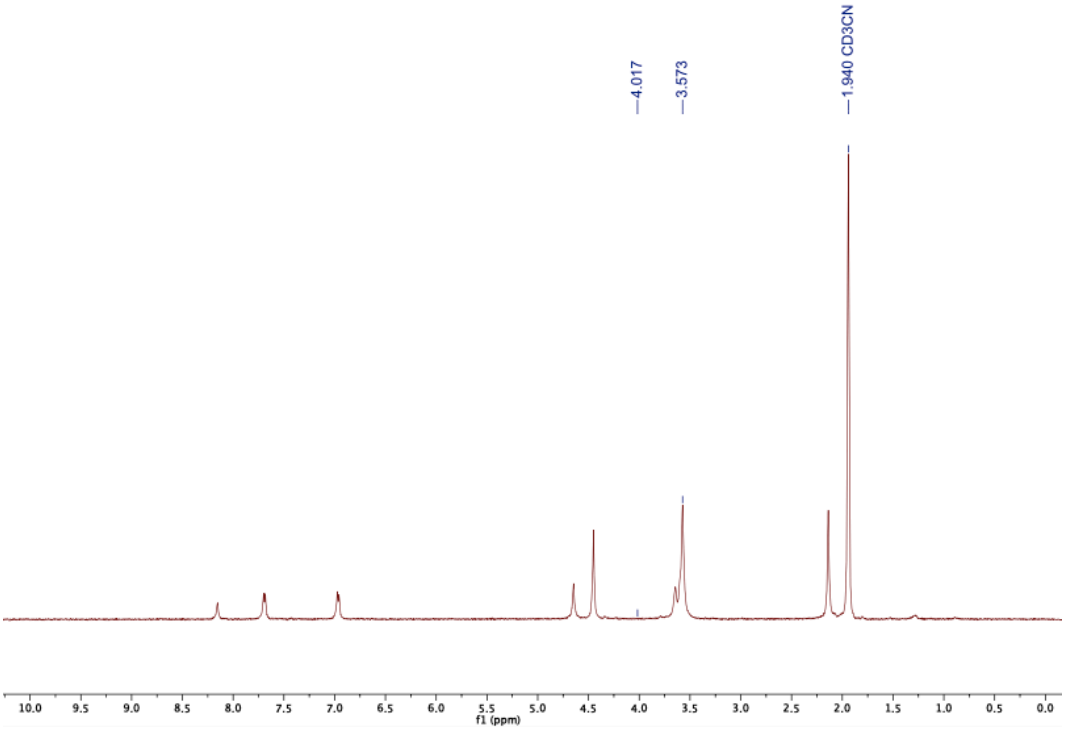

Figure S51. ^{1}H-NMR (500 MHz) of compound **8** + 0.5 equiv. of KPF_6 in CD_3CN.

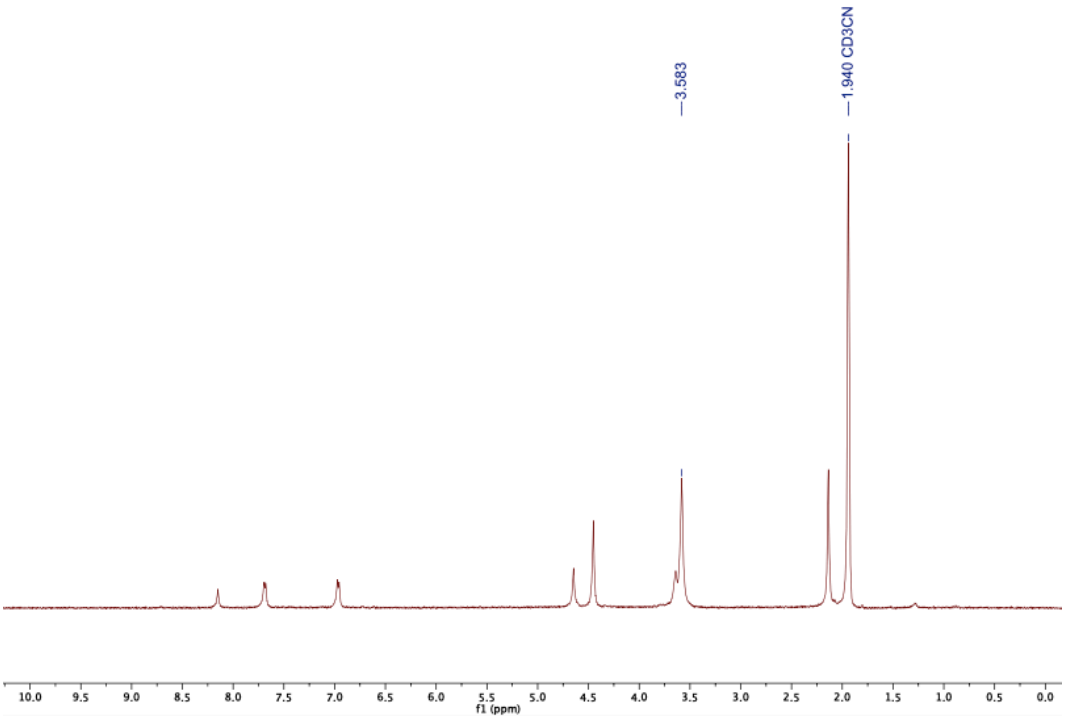

Figure S52. ^{1}H-NMR (500 MHz) of compound **8** + 0.7 equiv. of KPF_6 in CD_3CN.

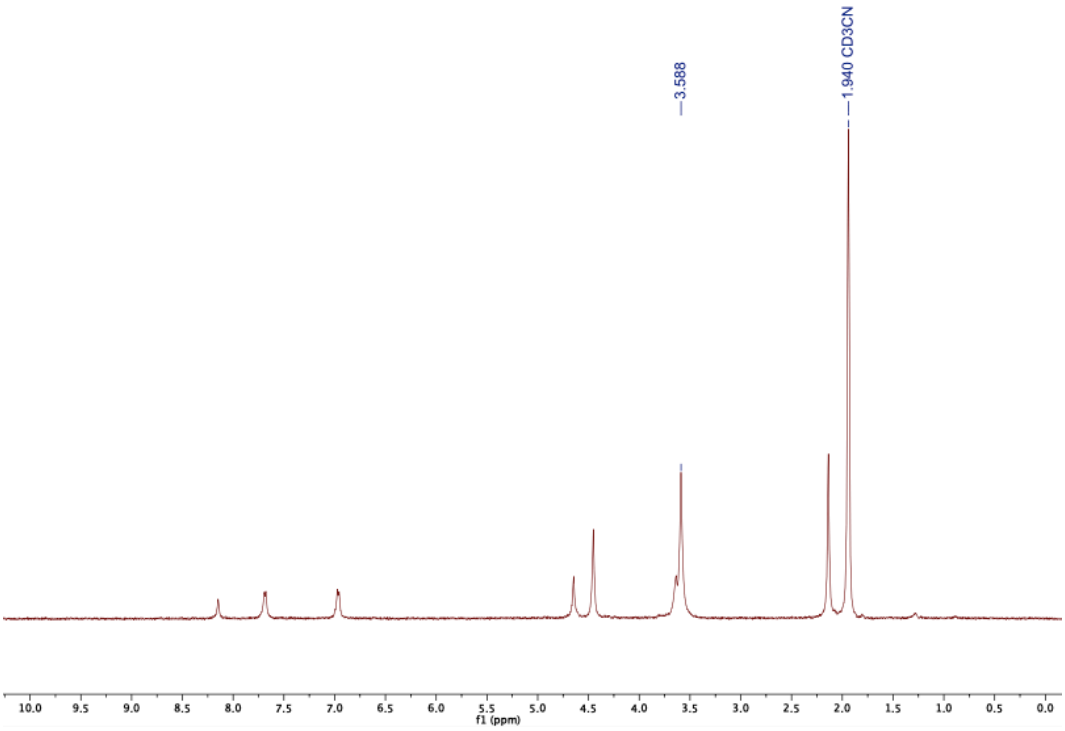

Figure S53. ^{1}H-NMR (500 MHz) of compound **8** + 0.9 equiv. of KPF_6 in CD_3CN.

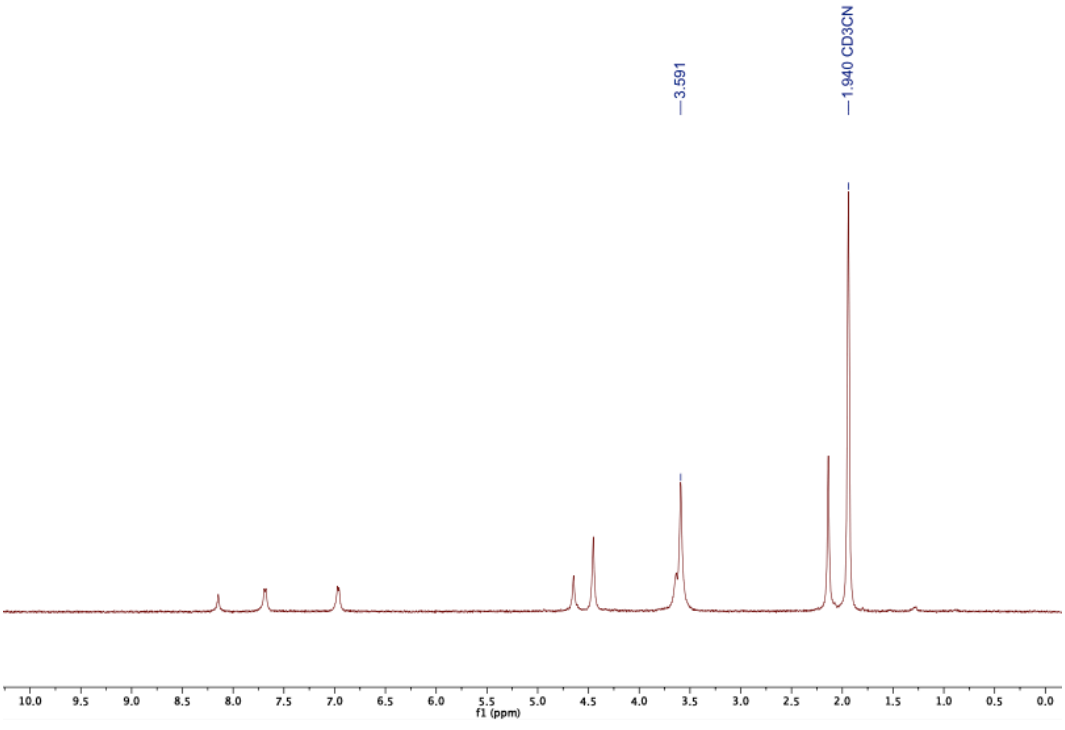

Figure S54. ^{1}H-NMR (500 MHz) of compound **8** + 1 equiv. of KPF_6 in CD_3CN.

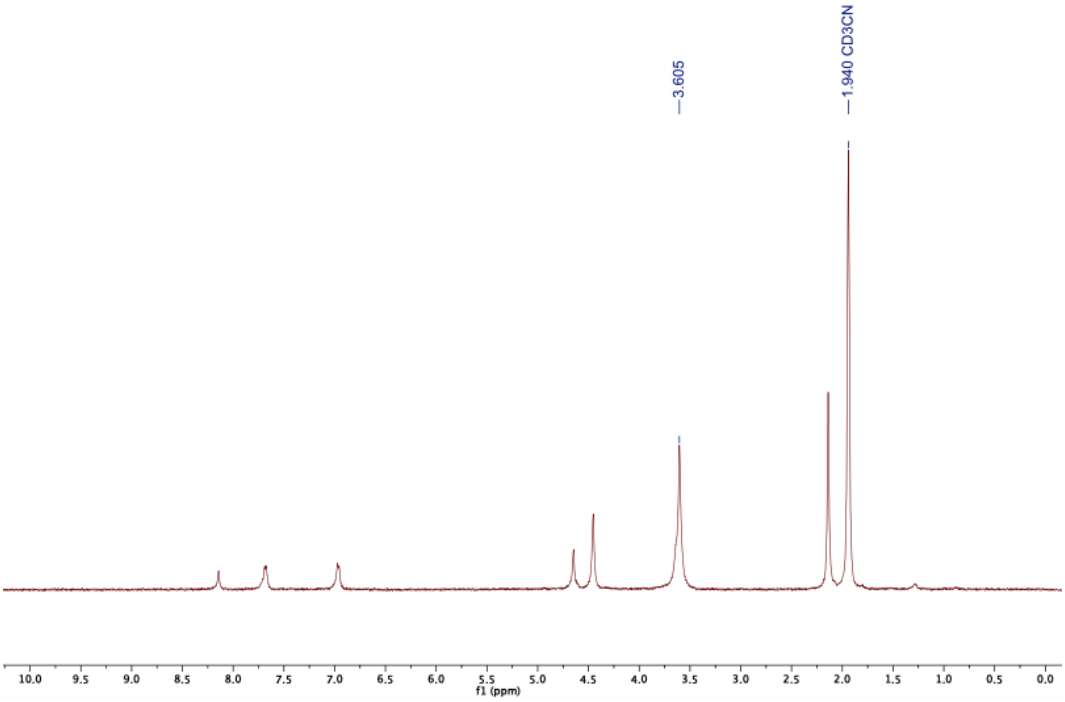

Figure S55. ^{1}H-NMR (500 MHz) of compound **8** + 2 equiv. of KPF_6 in CD_3CN.

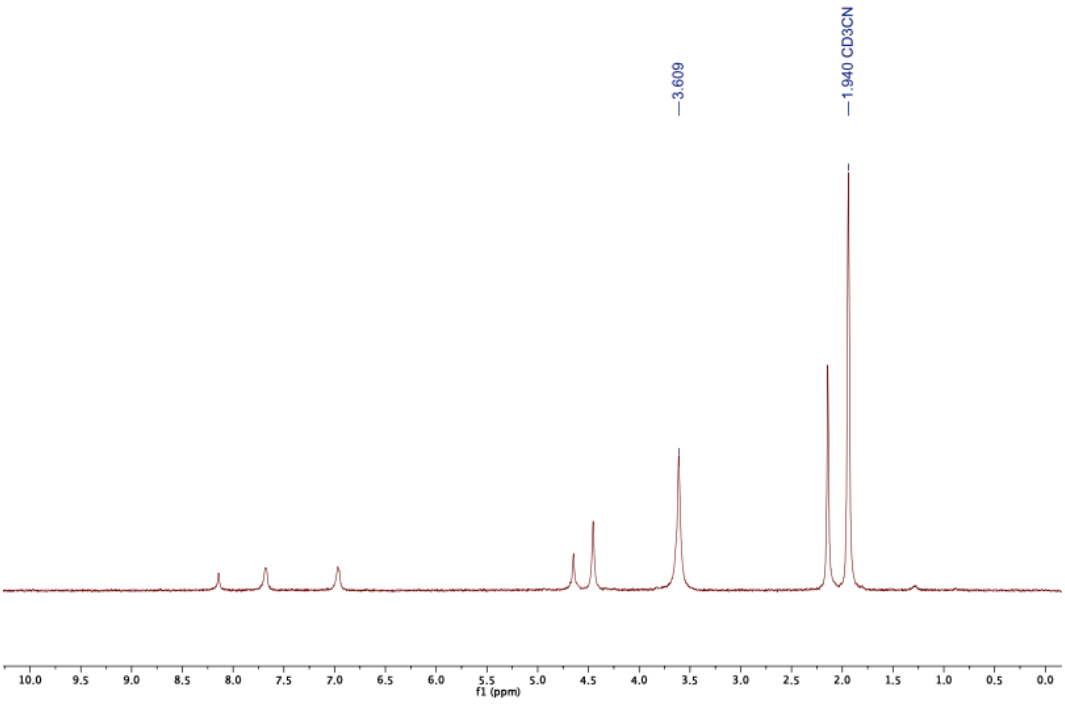

Figure S56. ^{1}H-NMR (500 MHz) of compound **8** + 4 equiv. of KPF_6 in CD_3CN.

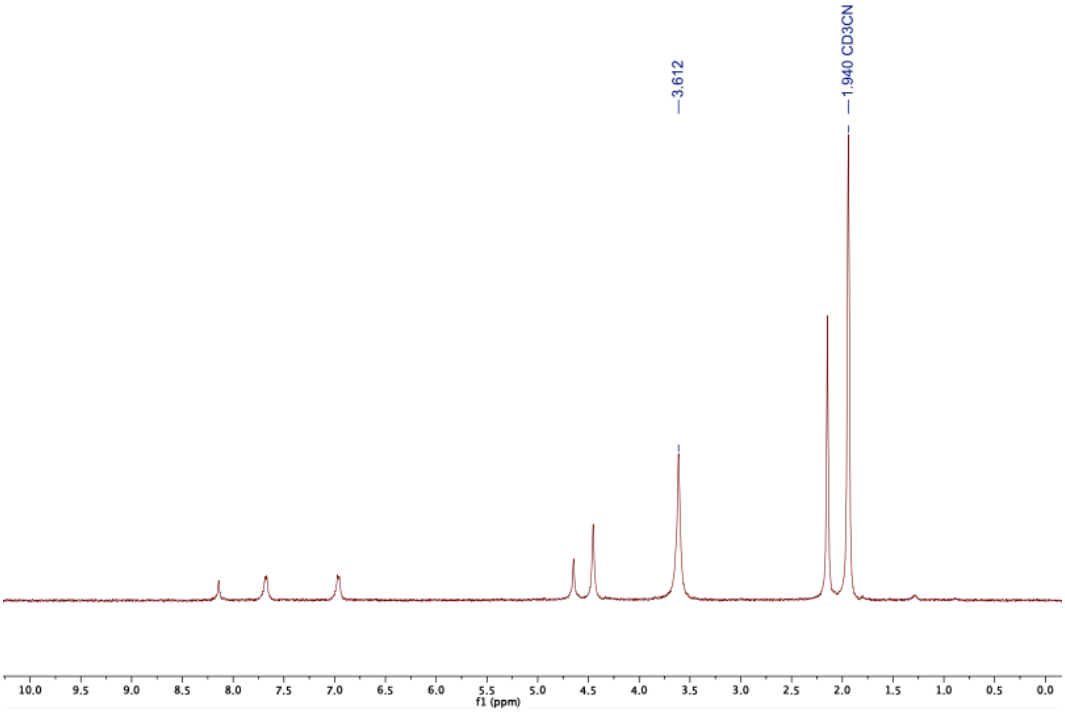

Figure S57. ^{1}H-NMR (500 MHz) of compound **8** + 6 equiv. of KPF_6 in CD_3CN.

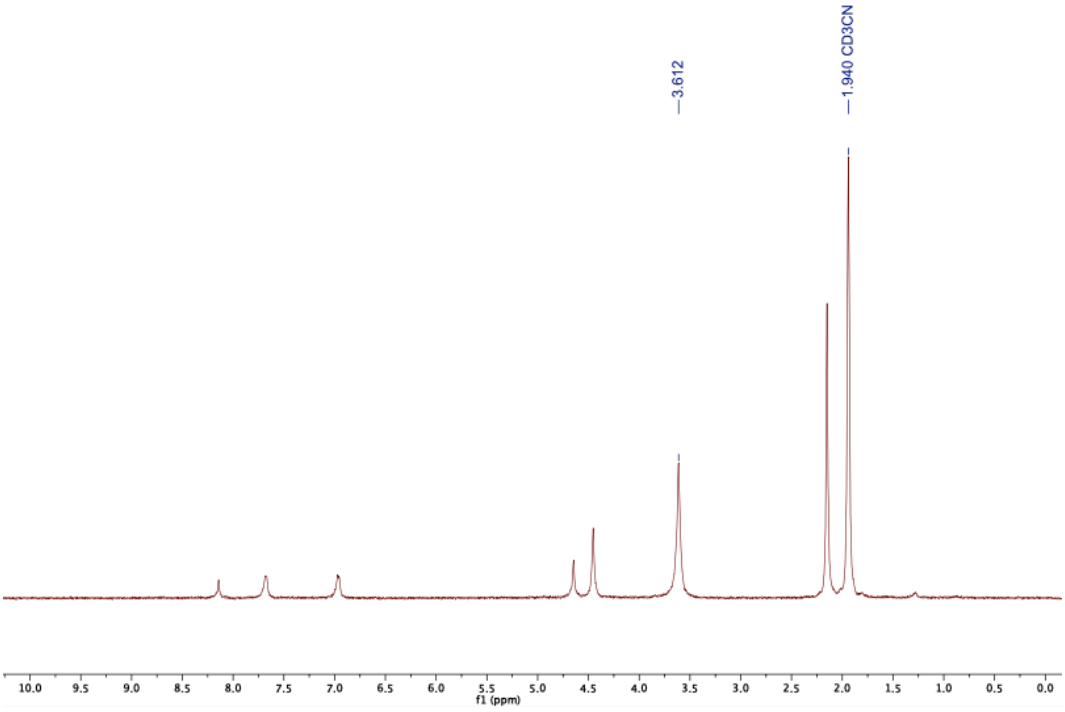

Figure S58. ^{1}H-NMR (500 MHz) of compound **8** + 8 equiv. of KPF_6 in CD_3CN.

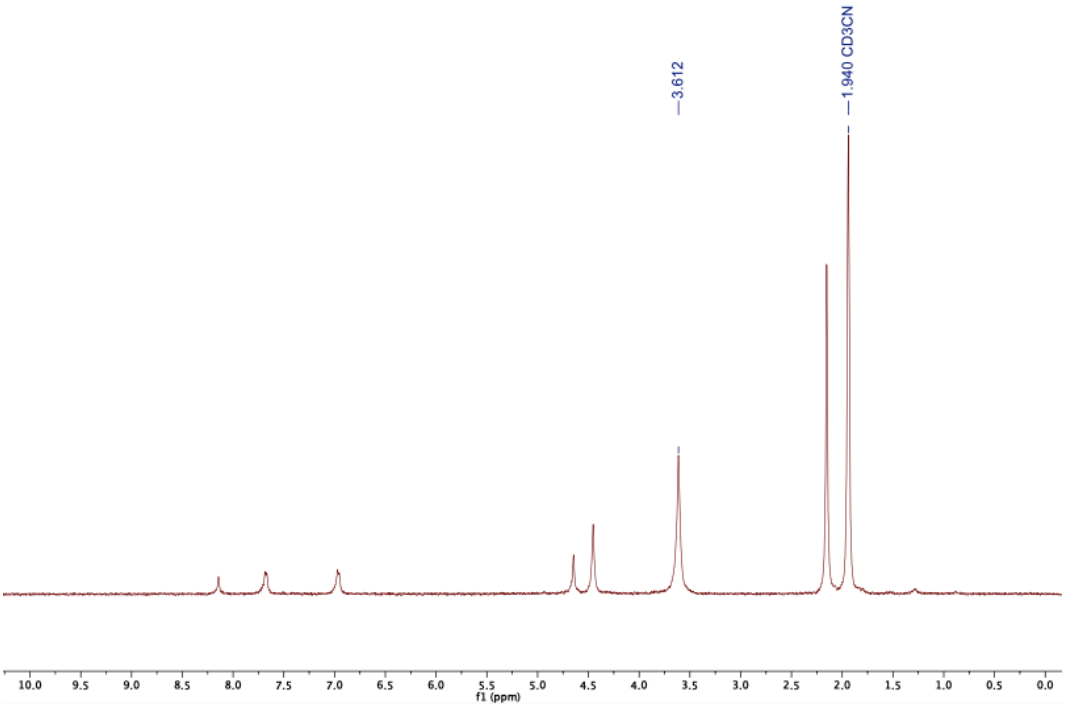

Figure S59. ^{1}H-NMR (500 MHz) of compound **8** + 10 equiv. of KPF_6 in CD_3CN.

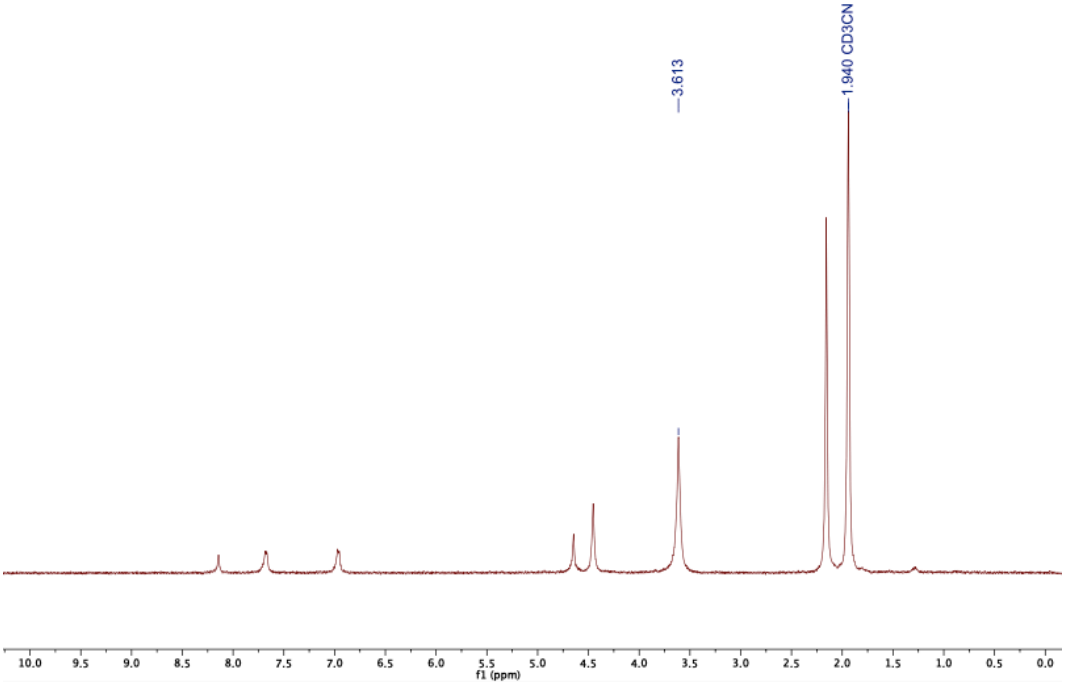

Figure S60. ^{1}H-NMR (500 MHz) of compound **8** + 12 equiv. of KPF_6 in CD_3CN.

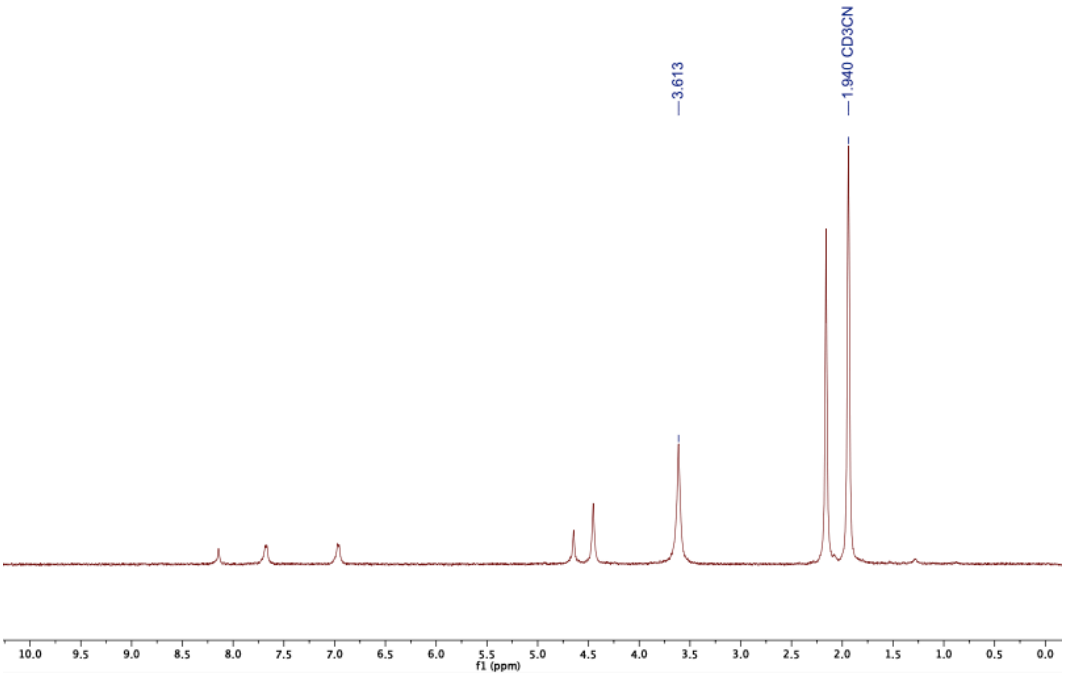

Figure S61. ^{1}H-NMR (500 MHz) of compound **8** + 14 equiv. of KPF_6 in CD_3CN.

S2. FTIR

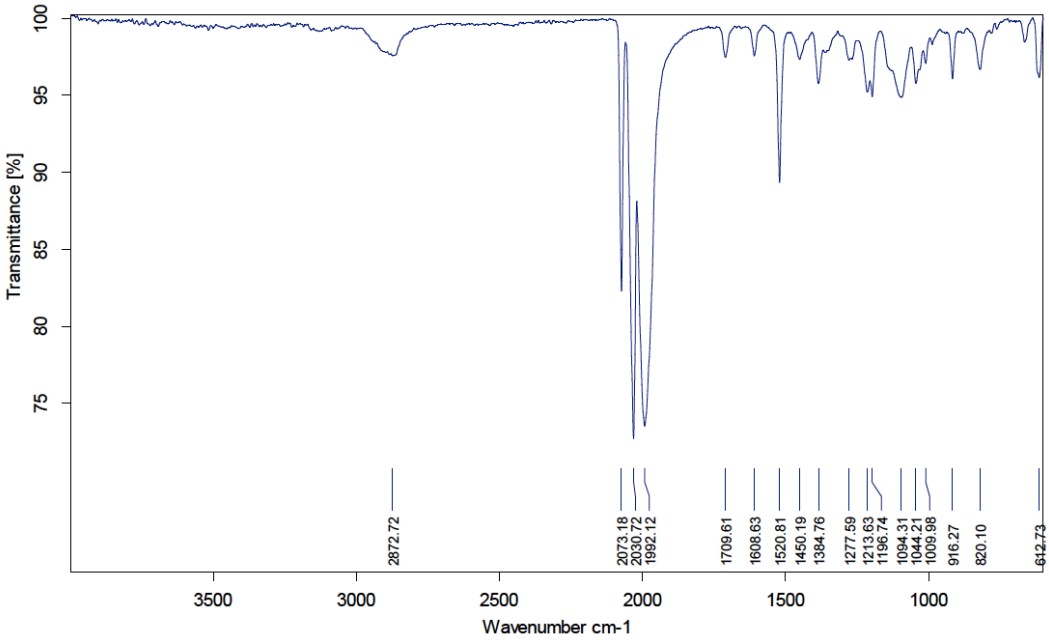

Figure S62. FTIR (film) of compound **7**.

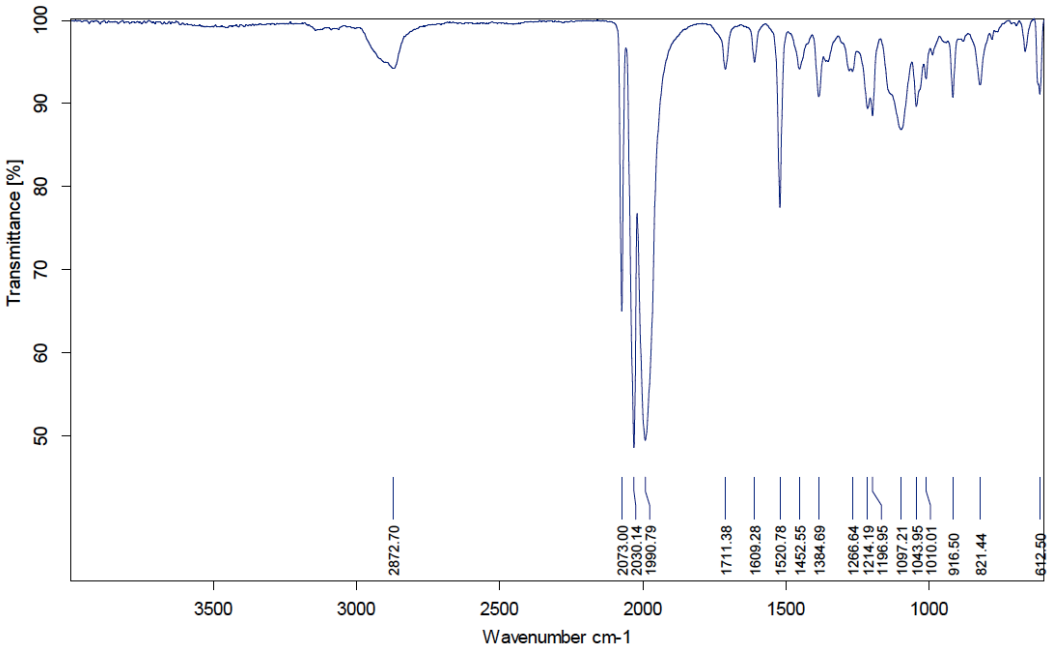

Figure S63. FTIR (film) of compound **8**.

S3. TOF calculations

The values of TOF were calculated using eqs 1-3 where i_{cat} is the catalytic current in the presence of acid, i_p is the peak current in the absence of acid, n is the number of electrons required to generate 1 mol of H_2 (here, $n = 2$), F is the Faraday constant, ν is the scan rate in Vs^{-1}, R is the ideal gas constant, T is the temperature in Kelvin and k_{obs} is the observed rate constant in s^{-1}.

$$\frac{i_{cat}}{i_p} = \frac{n}{0.4463} \cdot \frac{\sqrt{RT(k[H^+]^x)}}{F\nu} \quad (1)$$

$$k_{obs} = k[H^+]^x \quad (2)$$

$$k_{obs} = 1.94\, V^{-1} \cdot \nu \left(\frac{i_{cat}}{i_p}\right)^2 \quad (3)$$

S4:

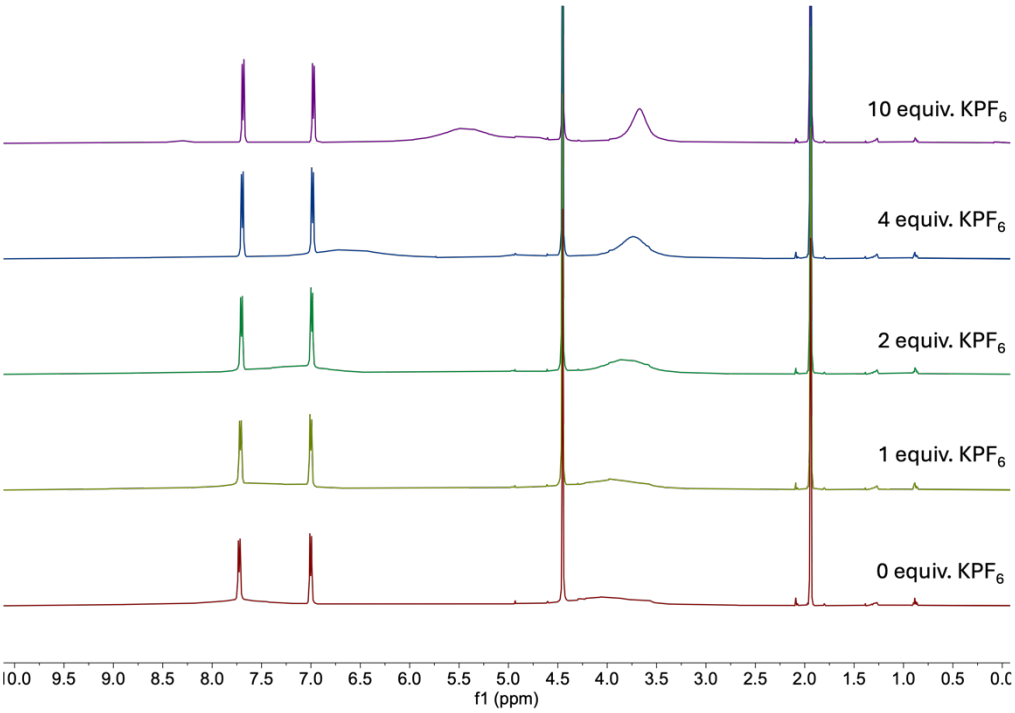

Figure S64. ^{1}H NMR spectra (500 MHz) of compound **8** with 5 equiv. of TFA and KPF_6 (0-10 equiv.) in CD_3CN at 25 ºC.

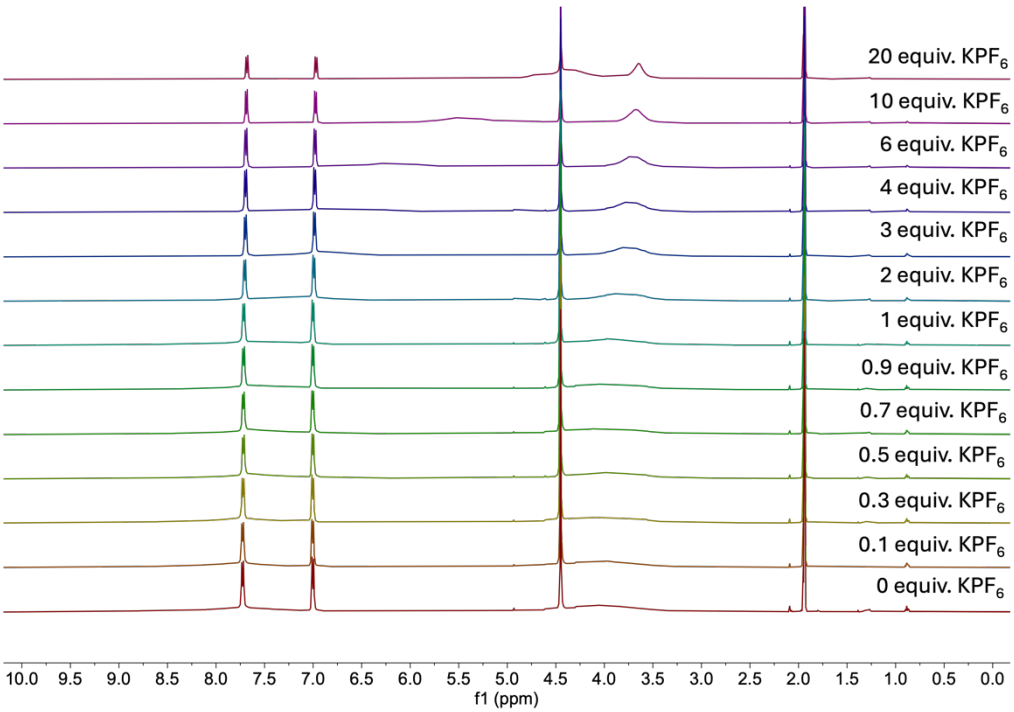

Figure S65. ^{1}H NMR spectra (500 MHz) of compound **8** with 5 equiv. of TFA and KPF_6 (0-20 equiv.) in CD_3CN at 25 ºC.

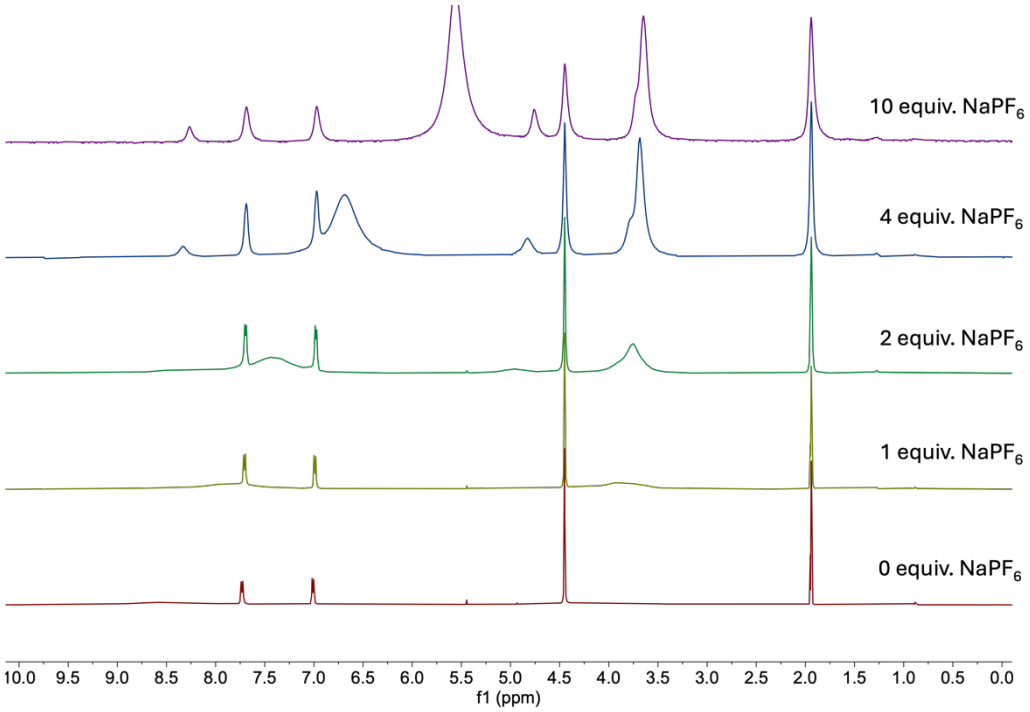

Figure S66. ^{1}H NMR spectra (500 MHz) of compound **8** with 5 equiv. of TFA and $NaPF_6$ (0-10 equiv.) in CD_3CN at 25 ºC.

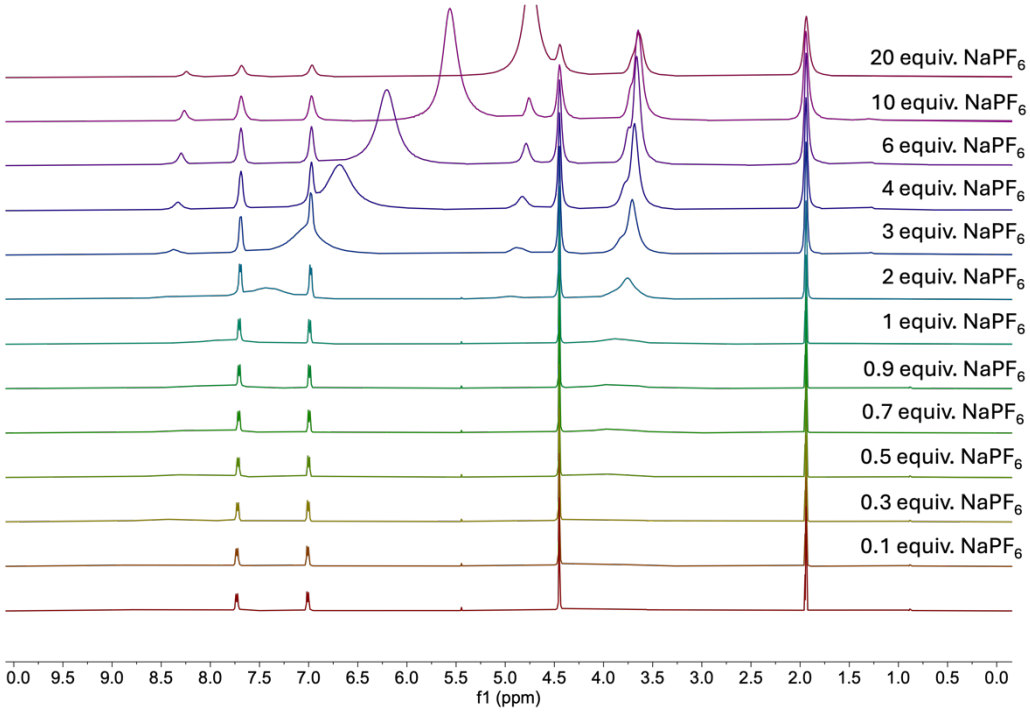

Figure S67. ^{1}H NMR spectra (500 MHz) of compound **8** with 5 equiv. of TFA and $NaPF_6$ (0-20 equiv.) in CD_3CN at 25 ºC.

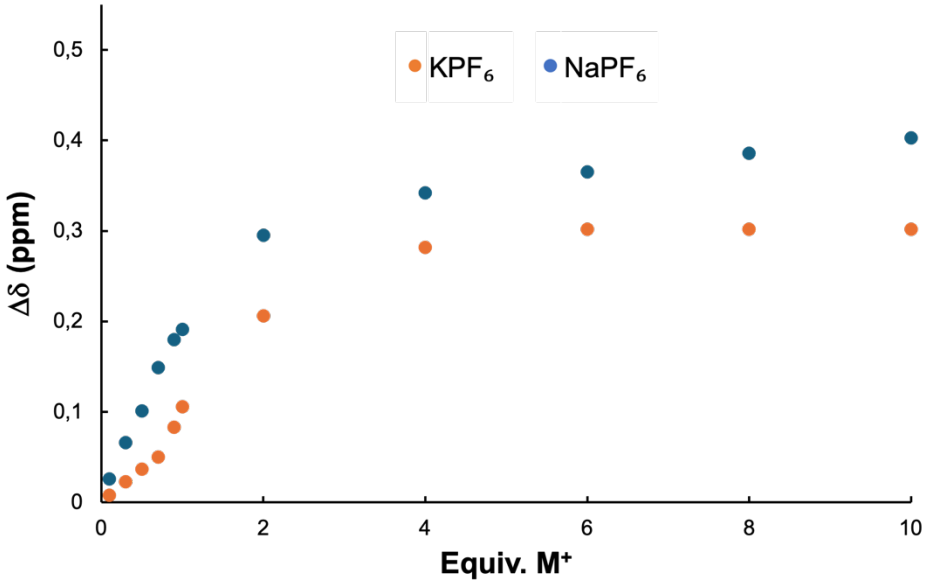

Figure S68. Representation of Δδ (ppm) vs equivalents of Na^+ and K^+ for **7** (left) and **8** (right) at 25 ºC.

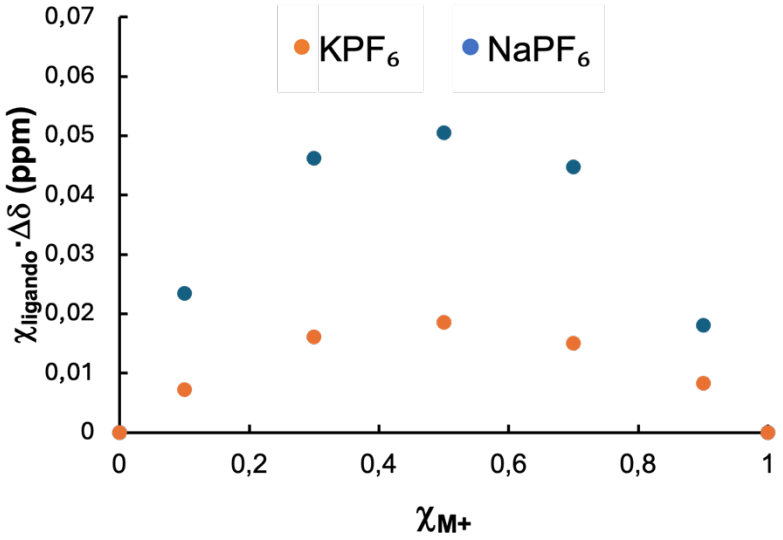

Figure S69. Job plots of compound **8** + 5 equiv. TFA with $NaPF_6$ and KPF_6 at 25 ºC.

Experimental *K*a values in CH_3CN:

[**8**-Na^+] 4.04 10^2 M^{-1}

[**8**-K^+] 1.26 10^3 M^{-1}

S5. Computational details

Cartesian coordinates and total electronic energies

114
Complex **[7-Na$^+$]**. E = -5588.344251
NImag=0

11	1.572028000	4.721470000	0.237139000
8	2.535580000	3.818564000	2.391255000
6	2.946648000	4.997820000	3.053499000
1	3.466868000	4.764247000	3.996523000
1	3.648630000	5.562547000	2.411622000
6	1.720853000	5.821896000	3.335638000
1	2.016003000	6.776949000	3.799079000
1	1.052573000	5.293305000	4.035961000
8	1.063300000	6.027897000	2.104925000
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6	-10.751942000	-1.305858000	-1.147272000
6	-9.785621000	-3.598930000	-0.513306000
6	-8.132074000	-0.630983000	-2.548212000
6	-5.776986000	-0.694815000	-1.279919000
6	-7.152782000	-2.899353000	-1.892809000

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1	4.054269000	2.734402000	-3.500379000
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7	5.029356000	3.420891000	-1.714813000
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1	8.935035000	-0.476617000	1.240497000
1	2.002030000	0.431906000	-0.576756000
1	1.856871000	4.497844000	-3.948101000

114
Complex **[7-K$^+$]**. E = -5454.351225
NImag=0

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1	4.289038000	2.474780000	2.940804000
6	2.459808000	3.239750000	3.784088000
1	2.861757000	3.561341000	4.758003000
1	1.427871000	2.882517000	3.945540000
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6	1.558887000	5.355121000	3.204424000
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1	2.043602000	6.312803000	2.974840000
6	0.270863000	5.258054000	2.423548000
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1	-0.159552000	4.239778000	2.505783000
8	0.544792000	5.570888000	1.071700000
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1	-1.334210000	6.301235000	0.582145000
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8	0.505035000	4.742413000	-1.712024000
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1	1.231538000	6.070652000	-3.144172000
6	1.119625000	0.608804000	-1.370309000
1	1.205388000	1.318374000	-2.204150000
8	2.218247000	0.873861000	-0.517098000
6	2.399883000	-0.111409000	0.483261000
1	1.432777000	-0.394877000	0.929489000
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6	3.289370000	0.449992000	1.557076000
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8	-9.694544000	1.341055000	-2.704691000
8	-5.741785000	-0.213039000	-1.826914000
8	-8.897873000	-2.777177000	-3.282116000
6	-11.242863000	-1.891489000	1.749879000
6	-11.733712000	-0.391377000	-0.475501000
6	-11.141336000	-2.874489000	-0.768927000
6	-9.231456000	0.480875000	-2.094758000
6	-6.807644000	-0.446024000	-1.460684000

6	-8.750267000	-2.004118000	-2.440847000
6	-7.660790000	-2.280156000	1.987715000
1	-8.431549000	-2.491970000	2.733914000
6	-8.242931000	-0.008139000	2.312333000
1	-8.974232000	-0.393916000	3.028026000
7	-7.199902000	-0.947334000	2.124854000
6	-5.948269000	-0.548932000	1.620352000
6	-5.632741000	0.809381000	1.444947000
6	-4.960769000	-1.499670000	1.316064000
6	-4.381396000	1.198596000	0.993808000
1	-6.363219000	1.589850000	1.632559000
6	-3.705616000	-1.109975000	0.878324000
1	-5.145707000	-2.562128000	1.433393000
6	-3.414779000	0.239706000	0.712754000
1	-4.161684000	2.252268000	0.845825000
1	-2.950745000	-1.866947000	0.679791000
6	-1.273382000	-0.033722000	-0.552350000
1	-1.504206000	-0.997392000	-0.985535000
6	-0.180752000	0.792672000	-0.657391000
7	-2.132076000	0.639408000	0.251642000
7	-1.600581000	1.815655000	0.637302000
7	-0.426698000	1.908918000	0.083365000
1	-6.866981000	-3.019595000	2.080907000
1	-7.881858000	0.957432000	2.664194000
26	6.192020000	-2.269543000	-0.432395000
26	8.139492000	-3.544454000	0.344281000
16	8.228875000	-2.209669000	-1.570686000
16	7.421060000	-1.625863000	1.469008000
8	10.959961000	-3.622166000	1.174427000
8	6.926940000	-5.072441000	2.531139000
8	8.197785000	-5.861651000	-1.448484000
8	4.173835000	-3.149879000	1.497533000
8	4.716505000	-0.114375000	-1.794077000
8	5.354581000	-4.278495000	-2.384210000
6	9.856611000	-3.585033000	0.849123000
6	7.407005000	-4.481258000	1.667363000
6	8.169087000	-4.955872000	-0.738199000
6	4.951495000	-2.792008000	0.725931000
6	5.325769000	-0.883677000	-1.194057000
6	5.679734000	-3.486100000	-1.613218000
6	9.226717000	-0.611846000	-1.184793000
1	10.189111000	-0.975577000	-0.813468000
6	8.686853000	-0.236482000	1.090509000
1	9.667252000	-0.675561000	1.290147000
7	8.634533000	0.259437000	-0.236263000
6	7.650854000	1.193813000	-0.606080000
6	6.831221000	1.792625000	0.366361000
6	7.471994000	1.569932000	-1.947910000
6	5.865955000	2.718238000	0.007309000
1	6.903944000	1.527037000	1.416357000
6	6.501704000	2.492563000	-2.306714000
1	8.080894000	1.142390000	-2.737479000
6	5.695825000	3.060348000	-1.328691000
1	5.224347000	3.151781000	0.774292000
1	6.367444000	2.767211000	-3.350628000
6	3.615248000	3.737658000	-2.541596000
1	3.562491000	2.861018000	-3.174911000
6	2.776002000	4.813360000	-2.347836000
7	4.637415000	3.945593000	-1.675415000
7	4.449493000	5.087894000	-0.979852000

7	3.328848000	5.610262000	-1.388670000
1	9.373462000	-0.147883000	-2.158828000
1	8.490490000	0.531506000	1.837303000
1	1.180413000	-0.406621000	-1.792184000
1	1.135266000	4.369430000	-3.639442000

121
Complex **[8-Na$^+$]**. E = -5742.041954
NImag=0

11	-0.497947000	3.190593000	-0.376990000
8	-2.262287000	1.522354000	-1.466128000
6	-3.097582000	2.246171000	-2.343966000
1	-3.804536000	1.570470000	-2.855171000
1	-3.678493000	2.997950000	-1.784513000
6	-2.232917000	2.919723000	-3.362745000
1	-2.864541000	3.430221000	-4.108698000
1	-1.621853000	2.168806000	-3.893355000
8	-1.389811000	3.847536000	-2.708602000
6	-0.486965000	4.437938000	-3.621624000
1	0.083537000	3.650354000	-4.144153000
1	-1.030647000	5.021332000	-4.383188000
6	0.456389000	5.331456000	-2.877932000
1	-0.091768000	6.134617000	-2.354216000
1	1.140630000	5.807916000	-3.599615000
8	1.171427000	4.545164000	-1.950584000
6	2.238585000	5.255089000	-1.358683000
1	3.038685000	5.438775000	-2.094519000
1	1.886292000	6.234960000	-0.991540000
6	2.763425000	4.447623000	-0.210394000
1	3.656050000	4.936035000	0.215342000
1	3.053613000	3.437377000	-0.551347000
8	1.732606000	4.361198000	0.746721000
6	2.074158000	3.564902000	1.855380000
1	2.248433000	2.520713000	1.538314000
1	2.998263000	3.925974000	2.337536000
6	0.940303000	3.650078000	2.835599000
1	0.858611000	4.676121000	3.232598000
1	1.125252000	2.971198000	3.685841000
8	-0.254082000	3.304571000	2.164394000
6	-1.378525000	3.403816000	3.003997000
1	-1.325980000	4.340858000	3.586187000
6	-0.154076000	0.267812000	1.629417000
1	0.091810000	0.893399000	2.498095000
8	-1.335144000	0.796811000	1.082864000
6	-1.996718000	-0.105301000	0.217973000
1	-1.276343000	-0.603780000	-0.451708000
1	-2.515696000	-0.886588000	0.797772000
6	-2.982055000	0.667031000	-0.606736000
1	-3.657165000	1.244135000	0.048719000
1	-3.604402000	-0.032876000	-1.192217000
26	9.242486000	-1.031315000	1.072558000
26	11.257589000	-1.687506000	-0.159059000
16	9.284468000	-2.940729000	-0.284682000
16	9.958695000	0.143576000	-0.821299000
8	12.557495000	-2.387300000	-2.703782000
8	13.198739000	0.259309000	0.855346000

8	12.319681000	-3.853418000	1.503927000
8	10.405853000	1.178685000	2.596200000
8	6.457408000	-0.297967000	1.676848000
8	9.524971000	-2.905245000	3.301179000
6	12.045909000	-2.114061000	-1.709507000
6	12.441797000	-0.513125000	0.459145000
6	11.910345000	-2.995154000	0.854133000
6	9.942052000	0.304882000	2.006387000
6	7.519163000	-0.598315000	1.349663000
6	9.409135000	-2.157956000	2.432430000
6	8.496931000	-2.635456000	-2.007421000
1	9.299267000	-2.838065000	-2.721730000
6	8.991800000	-0.353669000	-2.403847000
1	9.754610000	-0.730365000	-3.090524000
7	7.984718000	-1.329864000	-2.205163000
6	6.708271000	-0.972323000	-1.734311000
6	6.282789000	0.366962000	-1.748613000
6	5.810253000	-1.947029000	-1.269052000
6	5.010790000	0.714890000	-1.324919000
1	6.941093000	1.165130000	-2.075899000
6	4.534008000	-1.599634000	-0.855294000
1	6.088174000	-2.994460000	-1.219459000
6	4.134836000	-0.269068000	-0.879925000
1	4.703989000	1.757738000	-1.322088000
1	3.848969000	-2.372054000	-0.513833000
6	2.140671000	-0.431181000	0.616547000
1	2.522509000	-1.235239000	1.230839000
6	0.979305000	0.304252000	0.653139000
7	2.842665000	0.095202000	-0.416736000
7	2.157712000	1.089892000	-1.004049000
7	1.036130000	1.222709000	-0.349230000
1	7.736585000	-3.409203000	-2.105725000
1	8.601826000	0.585186000	-2.793226000
26	-7.910745000	-1.990482000	0.107052000
26	-10.203164000	-2.739394000	-0.360867000
16	-9.670468000	-1.558442000	1.583882000
16	-9.251446000	-0.954021000	-1.525907000
8	-13.039434000	-2.063022000	-0.739363000
8	-9.686868000	-4.353389000	-2.753318000
8	-10.571640000	-5.090093000	1.350217000
8	-6.404438000	-3.039198000	-2.170808000
8	-5.682216000	-0.389838000	1.172854000
8	-7.291535000	-4.319306000	1.763674000
6	-11.930647000	-2.332609000	-0.588155000
6	-9.896863000	-3.727657000	-1.809432000
6	-10.422439000	-4.173443000	0.669364000
6	-6.992297000	-2.636982000	-1.265765000
6	-6.599644000	-0.925154000	0.728100000
6	-7.533948000	-3.401458000	1.110274000
6	-10.333648000	0.240821000	1.425607000
1	-11.399394000	0.122529000	1.209797000
6	-10.073104000	0.661155000	-0.894158000
1	-11.149695000	0.481441000	-0.954966000
7	-9.713275000	1.031975000	0.425140000
6	-8.468962000	1.646009000	0.663204000
6	-7.608386000	1.968145000	-0.398087000
6	-8.061645000	1.966018000	1.967326000
6	-6.358555000	2.515382000	-0.160401000
1	-7.872447000	1.746092000	-1.426561000
6	-6.814661000	2.520513000	2.205228000

1	-8.710455000	1.786900000	2.818805000
6	-5.948043000	2.763128000	1.144338000
1	-5.687572000	2.704146000	-0.993130000
1	-6.518179000	2.754450000	3.224852000
6	-3.843760000	2.859661000	2.472684000
1	-4.206048000	2.275917000	3.307635000
6	-2.614149000	3.395075000	2.179773000
7	-4.612842000	3.174151000	1.401058000
7	-3.900529000	3.851562000	0.485290000
7	-2.688482000	3.986129000	0.957651000
1	-10.213930000	0.649845000	2.427099000
1	-9.799015000	1.419451000	-1.627951000
1	-0.302476000	-0.760712000	1.996185000
1	-1.406898000	2.575912000	3.733612000

121
Complex **[8-K$^+$]**. E = -5608.059441
NImag=0

19	-0.833419000	3.472687000	-0.368757000
8	-3.156321000	2.712447000	-1.766910000
6	-3.978965000	3.861080000	-1.789685000
1	-4.973362000	3.622768000	-2.203476000
1	-4.123055000	4.243522000	-0.762076000
6	-3.327129000	4.899150000	-2.656152000
1	-4.002856000	5.762131000	-2.778660000
1	-3.143146000	4.471265000	-3.656807000
8	-2.105857000	5.298591000	-2.069729000
6	-1.299002000	6.027684000	-2.969546000
1	-1.112377000	5.427990000	-3.877661000
1	-1.801956000	6.958648000	-3.281818000
6	0.006221000	6.369827000	-2.312755000
1	-0.162539000	6.974693000	-1.403998000
1	0.601848000	6.979832000	-3.012334000
8	0.688150000	5.177388000	-1.983636000
6	2.017414000	5.416562000	-1.568233000
1	2.641582000	5.715645000	-2.426502000
1	2.047320000	6.236384000	-0.829506000
6	2.568896000	4.166933000	-0.946234000
1	3.654998000	4.282151000	-0.789570000
1	2.412937000	3.304536000	-1.620230000
8	1.909793000	3.950296000	0.284514000
6	2.417337000	2.834761000	0.982536000
1	2.287870000	1.918343000	0.386021000
1	3.497919000	2.949570000	1.177914000
6	1.694010000	2.716668000	2.291885000
1	1.857110000	3.629163000	2.890709000
1	2.100154000	1.862898000	2.860463000
8	0.311923000	2.547925000	2.044660000
6	-0.453717000	2.640835000	3.230764000
1	-0.120177000	3.513512000	3.818035000
6	-1.105037000	0.019633000	0.624464000
1	-0.847275000	0.287037000	1.657732000
8	-2.061370000	0.954184000	0.193465000
6	-2.788581000	0.526645000	-0.945809000
1	-2.121844000	0.389903000	-1.812637000
1	-3.282142000	-0.438570000	-0.743458000
6	-3.815057000	1.575720000	-1.249878000

1	-4.352643000	1.827006000	-0.320316000
1	-4.556253000	1.193239000	-1.973937000
26	8.356821000	-0.888744000	1.019917000
26	10.486654000	-1.630286000	0.064826000
16	8.579498000	-2.983202000	-0.007052000
16	9.183808000	0.004842000	-0.986457000
8	12.015889000	-2.681648000	-2.217296000
8	12.262027000	0.556799000	0.870132000
8	11.479177000	-3.430185000	2.152942000
8	9.321486000	1.590760000	2.234136000
8	5.497286000	-0.262485000	1.327911000
8	8.569135000	-2.360532000	3.537715000
6	11.415636000	-2.269942000	-1.325704000
6	11.572238000	-0.311390000	0.559005000
6	11.098217000	-2.716202000	1.333568000
6	8.931413000	0.613199000	1.766136000
6	6.596712000	-0.528639000	1.115425000
6	8.479327000	-1.771565000	2.551803000
6	7.913943000	-2.994865000	-1.807432000
1	8.772023000	-3.282174000	-2.421128000
6	8.372151000	-0.787218000	-2.534809000
1	9.200878000	-1.238900000	-3.086886000
7	7.382083000	-1.760503000	-2.255782000
6	6.065044000	-1.378066000	-1.942673000
6	5.651281000	-0.041611000	-2.071200000
6	5.116861000	-2.327211000	-1.527105000
6	4.345107000	0.329730000	-1.797613000
1	6.348385000	0.739252000	-2.357286000
6	3.806825000	-1.958344000	-1.267129000
1	5.377231000	-3.374250000	-1.412957000
6	3.421324000	-0.629065000	-1.396151000
1	4.050754000	1.373467000	-1.873254000
1	3.084892000	-2.714508000	-0.968032000
6	1.257858000	-0.751872000	-0.147503000
1	1.529835000	-1.588238000	0.481304000
6	0.136726000	0.043622000	-0.213677000
7	2.093090000	-0.237230000	-1.083842000
7	1.528217000	0.811440000	-1.704127000
7	0.347826000	0.985332000	-1.171263000
1	7.185345000	-3.803462000	-1.820156000
1	7.984699000	0.055456000	-3.106775000
26	-6.768784000	-1.943858000	-0.167234000
26	-8.948449000	-2.955172000	-0.665287000
16	-8.224628000	-2.613974000	1.530580000
16	-8.583241000	-0.670048000	-0.979696000
8	-11.874928000	-2.894298000	-0.382429000
8	-8.671852000	-3.231651000	-3.569371000
8	-8.566174000	-5.822569000	-0.198575000
8	-5.622253000	-1.550709000	-2.832721000
8	-4.659280000	-0.550454000	1.336498000
8	-5.447297000	-4.530200000	0.163582000
6	-10.729463000	-2.924129000	-0.491537000
6	-8.783814000	-3.133325000	-2.427281000
6	-8.710435000	-4.696505000	-0.391386000
6	-6.060766000	-1.706758000	-1.779223000
6	-5.546705000	-0.998796000	0.755575000
6	-5.968486000	-3.511183000	0.028470000
6	-9.183754000	-1.134016000	2.303585000
1	-10.235940000	-1.414900000	2.205492000
6	-9.535020000	0.249842000	0.412823000

1	-10.541297000	-0.176376000	0.411537000
7	-8.953151000	0.128875000	1.700312000
6	-7.790860000	0.865146000	2.003375000
6	-7.322292000	1.859637000	1.129524000
6	-7.068781000	0.630291000	3.182794000
6	-6.117091000	2.499459000	1.362454000
1	-7.857336000	2.115760000	0.221129000
6	-5.858937000	1.265793000	3.412953000
1	-7.419936000	-0.079282000	3.924943000
6	-5.352220000	2.154258000	2.471336000
1	-5.745078000	3.226630000	0.646236000
1	-5.297383000	1.032953000	4.314319000
6	-2.965903000	2.005555000	3.174566000
1	-3.056432000	1.083198000	3.731467000
6	-1.885575000	2.794993000	2.868390000
7	-4.013876000	2.615538000	2.570980000
7	-3.606830000	3.714160000	1.907165000
7	-2.321659000	3.825217000	2.092074000
1	-8.903266000	-1.161776000	3.355284000
1	-9.592131000	1.283820000	0.073756000
1	-1.532684000	-0.997053000	0.646223000
1	-0.316907000	1.748326000	3.863485000

125
Complex **[8H4-K]**. E = -5609.677753
NImag=0

6	-3.729495000	0.148250000	1.638940000
7	-3.614748000	0.994817000	0.585344000
6	-5.058643000	0.210496000	1.973702000
7	-4.735348000	1.574822000	0.243930000
7	-5.611349000	1.092859000	1.097819000
1	-5.626977000	-0.309797000	2.731735000
6	-6.975759000	1.510963000	1.004682000
6	-7.770949000	1.483758000	2.141323000
6	-7.466801000	1.930209000	-0.223959000
6	-9.095986000	1.885943000	2.046041000
6	-8.787888000	2.341944000	-0.313927000
6	-9.594607000	2.306990000	0.818183000
1	-7.370398000	1.172386000	3.101558000
1	-9.696695000	1.876781000	2.949116000
1	-9.153177000	2.670777000	-1.280072000
26	-13.788486000	0.406278000	-0.518125000
26	-11.548165000	-0.571195000	-0.415305000
16	-11.966580000	1.439709000	-1.543455000
16	-12.503525000	0.509658000	1.427622000
7	-10.982280000	2.852361000	0.747532000
6	-14.923106000	1.787990000	-0.314154000
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