**Supplementary Information**

Syntheses, X-ray structure, emission and vibrational spectroscopies, DFT and thermogravimetric studies of two complexes containing the bidentate ligand 5-phenyl-1H-pyrazol-3-yl)methyl) phosphine oxide

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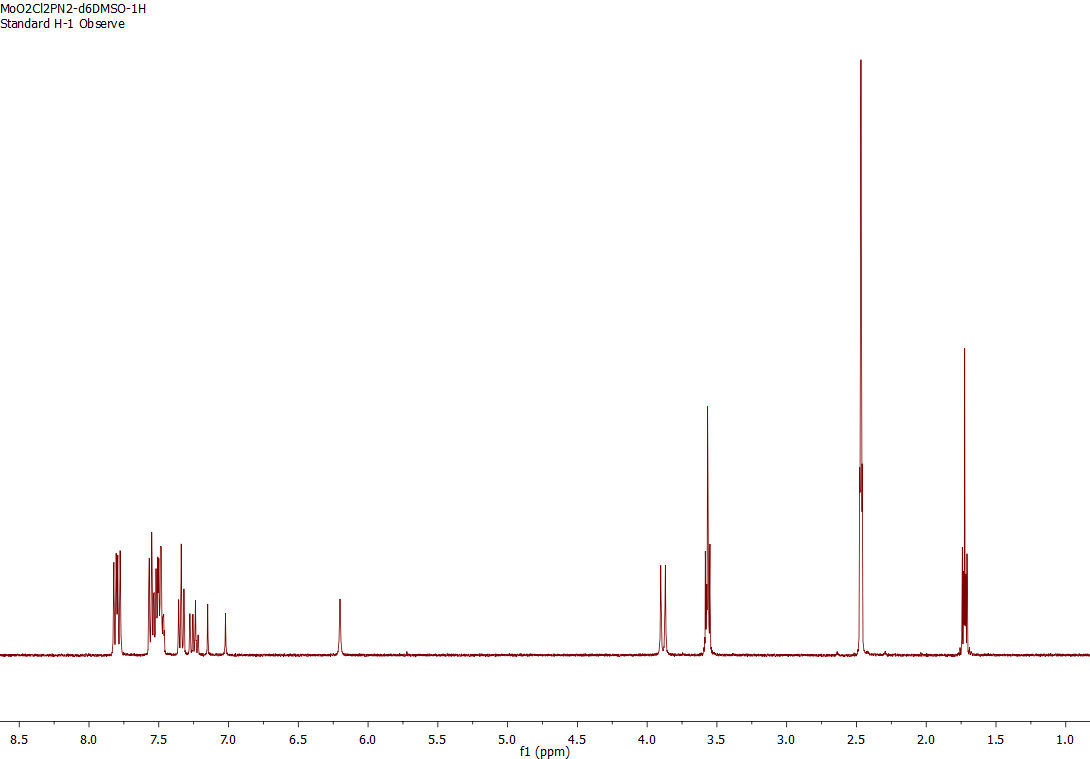
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## **Figure S1**. 1H NMR spectrum of complex **3** in (CD3)2SO.

[Co((C6H5)2POCH2(C3N2H2)(C6H5))2(C4H8O)2][ClO4]2

## **Figure S2**. TGA for Complex **2** under nitrogen.

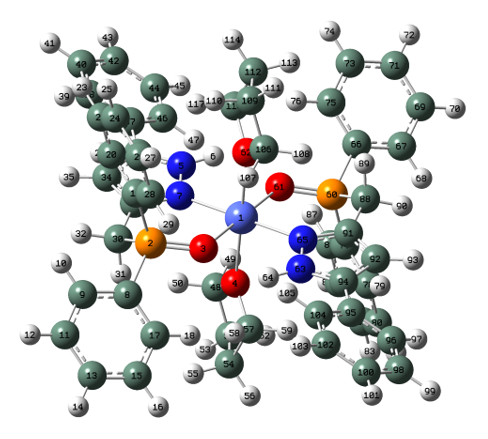
[Co((C6H5)2POCH2(C3N2H2)(C6H5))2(C4H8O)2][ClO4]2

## Figure S3. TGA for Complex 2 under oxygen.

## Figure S4. TGA for Co(ClO4)2•6H2O under nitrogen.

## **Figure S5**. TGA for Complex **3** under nitrogen.

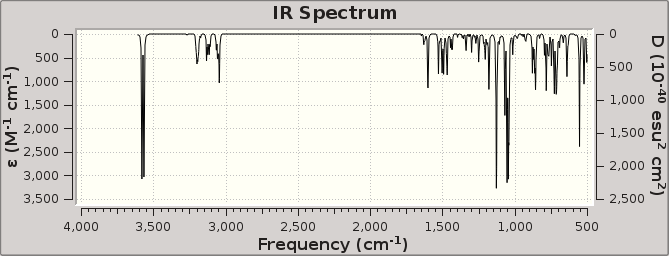
Theoretical Calculations.

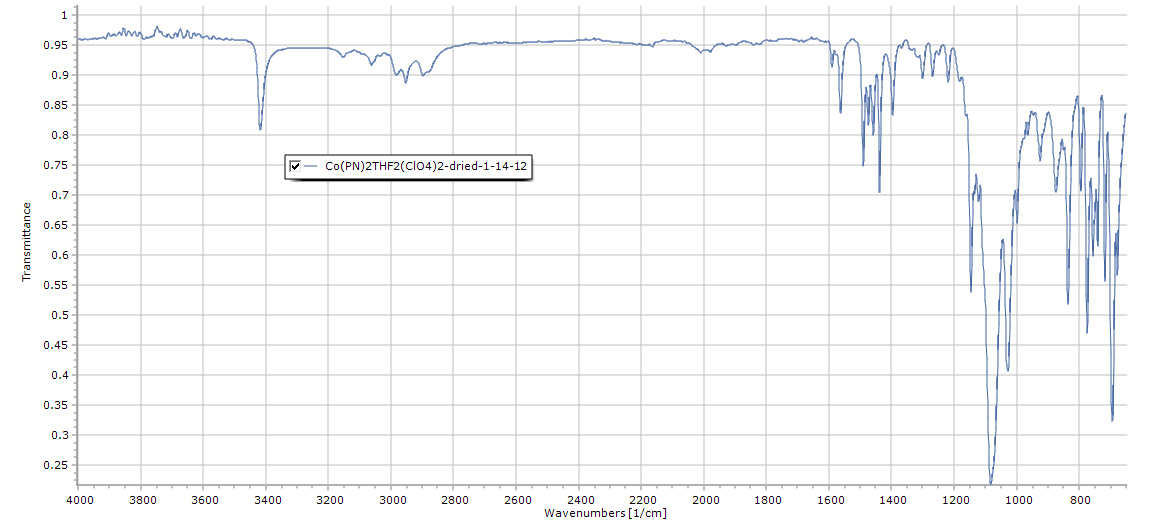


## **Figure S6**. Drawing of compound **2** with atoms represented as spheres of arbitrary size (H-white, C-grey, N-blue and O-red) using the GaussView [1] program.

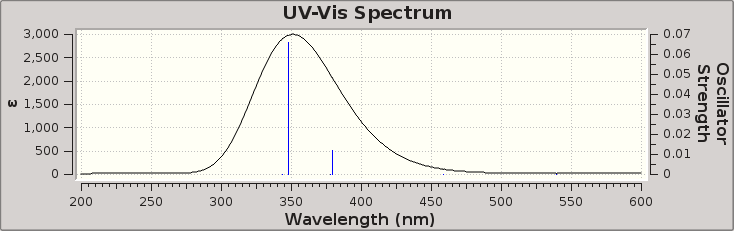
## **Table S1**. Atomic coordinates for **2**.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Row** | **Symbol** | **X** | **Y** | **Z** |
| 1 | Co | -0.01866 | -0.00152 | -0.01933 |
| 2 | P | 2.381864 | 2.171229 | 0.512861 |
| 3 | O | 1.986164 | 0.717375 | 0.2047 |
| 4 | O | 0.011928 | -0.66317 | 2.057006 |
| 5 | N | -2.1621 | 2.054374 | 0.533009 |
| 6 | H | -2.74216 | 1.309899 | 0.163748 |
| 7 | N | -0.84452 | 1.806112 | 0.659961 |
| 8 | C | 3.935363 | 2.218087 | 1.450366 |
| 9 | C | 4.621876 | 3.425973 | 1.636572 |
| 10 | H | 4.260932 | 4.342892 | 1.184861 |
| 11 | C | 5.787088 | 3.450705 | 2.396672 |
| 12 | H | 6.316373 | 4.38533 | 2.537954 |
| 13 | C | 6.276182 | 2.275248 | 2.966651 |
| 14 | H | 7.186542 | 2.297669 | 3.554063 |
| 15 | C | 5.599555 | 1.071947 | 2.777926 |
| 16 | H | 5.981672 | 0.157333 | 3.215399 |
| 17 | C | 4.428693 | 1.040827 | 2.023916 |
| 18 | H | 3.905391 | 0.105355 | 1.873887 |
| 19 | C | 2.628094 | 3.190312 | -0.97049 |
| 20 | C | 1.775218 | 4.250399 | -1.30051 |
| 21 | H | 0.930355 | 4.50056 | -0.67163 |
| 22 | C | 2.009165 | 5.000372 | -2.45164 |
| 23 | H | 1.349096 | 5.823128 | -2.69873 |
| 24 | C | 3.08853 | 4.695417 | -3.27759 |
| 25 | H | 3.270578 | 5.283023 | -4.16965 |
| 26 | C | 3.93879 | 3.636766 | -2.95593 |
| 27 | H | 4.780779 | 3.400946 | -3.59552 |
| 28 | C | 3.71326 | 2.886848 | -1.80672 |
| 29 | H | 4.387823 | 2.075585 | -1.55707 |
| 30 | C | 1.134653 | 2.982646 | 1.599922 |
| 31 | H | 1.259548 | 2.477734 | 2.564059 |
| 32 | H | 1.43478 | 4.020441 | 1.756076 |
| 33 | C | -0.30621 | 2.915235 | 1.182171 |
| 34 | C | -1.30187 | 3.886736 | 1.372098 |
| 35 | H | -1.17929 | 4.867952 | 1.799388 |
| 36 | C | -2.49444 | 3.299084 | 0.951205 |
| 37 | C | -3.86892 | 3.811051 | 0.934979 |
| 38 | C | -4.09979 | 5.187253 | 0.794401 |
| 39 | H | -3.26232 | 5.864772 | 0.678505 |
| 40 | C | -5.39853 | 5.684903 | 0.782175 |
| 41 | H | -5.56337 | 6.749999 | 0.670057 |
| 42 | C | -6.48395 | 4.818225 | 0.906261 |
| 43 | H | -7.49496 | 5.207955 | 0.895522 |
| 44 | C | -6.26382 | 3.448942 | 1.048234 |
| 45 | H | -7.10259 | 2.771342 | 1.155668 |
| 46 | C | -4.96637 | 2.946853 | 1.066578 |
| 47 | H | -4.81063 | 1.883914 | 1.21187 |
| 48 | C | -0.97879 | -0.28059 | 3.057246 |
| 49 | H | -1.96228 | -0.36587 | 2.599071 |
| 50 | H | -0.79935 | 0.760532 | 3.339207 |
| 51 | C | -0.7488 | -1.22888 | 4.226916 |
| 52 | H | -1.29235 | -2.16361 | 4.072885 |
| 53 | H | -1.07107 | -0.79389 | 5.173798 |
| 54 | C | 0.766053 | -1.46902 | 4.15899 |
| 55 | H | 1.306859 | -0.63206 | 4.608596 |
| 56 | H | 1.078089 | -2.386 | 4.660063 |
| 57 | C | 1.022505 | -1.52586 | 2.656175 |
| 58 | H | 2.000308 | -1.14526 | 2.365876 |
| 59 | H | 0.88877 | -2.53342 | 2.255457 |
| 60 | P | -2.39702 | -2.20216 | -0.49823 |
| 61 | O | -2.01673 | -0.73334 | -0.24694 |
| 62 | O | -0.03362 | 0.681489 | -2.08609 |
| 63 | N | 2.139024 | -2.02907 | -0.59196 |
| 64 | H | 2.70917 | -1.26722 | -0.24051 |
| 65 | N | 0.814193 | -1.80802 | -0.69511 |
| 66 | C | -3.96584 | -2.30522 | -1.40587 |
| 67 | C | -4.63511 | -3.52966 | -1.54019 |
| 68 | H | -4.25128 | -4.42558 | -1.06582 |
| 69 | C | -5.81258 | -3.5983 | -2.27836 |
| 70 | H | -6.32833 | -4.54561 | -2.37956 |
| 71 | C | -6.33093 | -2.45048 | -2.87807 |
| 72 | H | -7.25078 | -2.5072 | -3.44815 |
| 73 | C | -5.67094 | -1.23104 | -2.7417 |
| 74 | H | -6.07518 | -0.33787 | -3.20299 |
| 75 | C | -4.48807 | -1.1563 | -2.00967 |
| 76 | H | -3.97662 | -0.20894 | -1.90095 |
| 77 | C | -2.60381 | -3.17531 | 1.022278 |
| 78 | C | -1.73651 | -4.21922 | 1.366302 |
| 79 | H | -0.90043 | -4.48088 | 0.730406 |
| 80 | C | -1.94574 | -4.9412 | 2.539913 |
| 81 | H | -1.27473 | -5.75196 | 2.796988 |
| 82 | C | -3.01441 | -4.62431 | 3.375096 |
| 83 | H | -3.17743 | -5.1906 | 4.284469 |
| 84 | C | -3.87867 | -3.58138 | 3.039879 |
| 85 | H | -4.71284 | -3.33623 | 3.686203 |
| 86 | C | -3.67824 | -2.85987 | 1.867982 |
| 87 | H | -4.36639 | -2.06341 | 1.608374 |
| 88 | C | -1.16064 | -3.03636 | -1.58037 |
| 89 | H | -1.31387 | -2.57161 | -2.56043 |
| 90 | H | -1.44865 | -4.08384 | -1.68992 |
| 91 | C | 0.287647 | -2.9323 | -1.19675 |
| 92 | C | 1.298495 | -3.88532 | -1.39838 |
| 93 | H | 1.186895 | -4.87287 | -1.81395 |
| 94 | C | 2.487134 | -3.2709 | -1.00553 |
| 95 | C | 3.870371 | -3.75901 | -1.00941 |
| 96 | C | 4.126232 | -5.13085 | -0.86878 |
| 97 | H | 3.302014 | -5.82193 | -0.73861 |
| 98 | C | 5.43304 | -5.60702 | -0.87445 |
| 99 | H | 5.617035 | -6.66893 | -0.76199 |
| 100 | C | 6.502057 | -4.72292 | -1.01678 |
| 101 | H | 7.519446 | -5.09585 | -1.01987 |
| 102 | C | 6.257114 | -3.3579 | -1.15901 |
| 103 | H | 7.082841 | -2.66677 | -1.28047 |
| 104 | C | 4.95139 | -2.87735 | -1.15944 |
| 105 | H | 4.776167 | -1.81762 | -1.30486 |
| 106 | C | 0.999495 | 0.341431 | -3.05852 |
| 107 | H | 1.96453 | 0.457088 | -2.56918 |
| 108 | H | 0.864684 | -0.70255 | -3.35339 |
| 109 | C | 0.771569 | 1.291491 | -4.22685 |
| 110 | H | 1.27414 | 2.244561 | -4.04697 |
| 111 | H | 1.140611 | 0.878474 | -5.16646 |
| 112 | C | -0.75291 | 1.472411 | -4.20624 |
| 113 | H | -1.24534 | 0.618712 | -4.67945 |
| 114 | H | -1.08457 | 2.380728 | -4.71046 |
| 115 | C | -1.06003 | 1.506144 | -2.71191 |
| 116 | H | -2.03081 | 1.08394 | -2.45645 |
| 117 | H | -0.98204 | 2.515643 | -2.30107 |





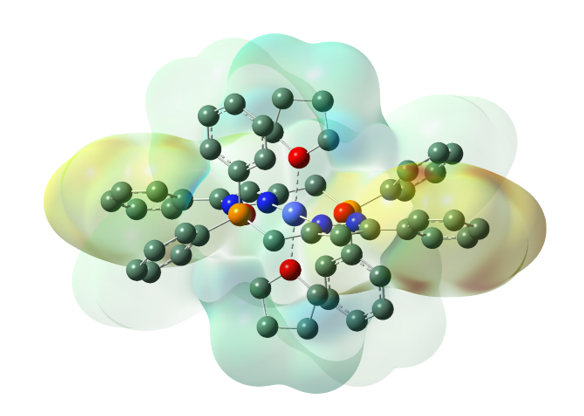
## **Figure S7**. Uncorrected calculated FTIR (top) and experimental (neat) spectrum of compound **2**.



## **Figure S8**. Calculated UV-Vis spectrum for 2.

## **Figure S9**. UV-vis absorption spectrum of **2** in CH2Cl2.

## **Figure S10**. Emission spectrum of **2** in CH2Cl2.

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## **Figure S11**. Difference density illustrations as iso-surfaces of complex **2** featuring excited state 9. Red areas indicate values for the different density of -4.575e-5 and blue are for 4.575e+5, see scale on top of illustration.

## **Table S2**. Excitation energies and oscillator strength for complex **2**

Of the 10 Excited States calculated, numbers 1-6 all had f=0 and are not listed.

Excited State 7: 3.2699 eV 379.17 nm f=0.0120 <S\*\*2>=5.360

235A -> 249A 0.12356

236A -> 239A 0.32756

236A -> 241A 0.16219

237A -> 238A 0.38446

232B -> 249B -0.12313

233B -> 235B 0.51914

233B -> 240B -0.32932

234B -> 237B 0.39114

Excited state symmetry could not be determined.

Excited State 8: 3.2827 eV 377.69 nm f=0.0002 <S\*\*2>=5.472

234A -> 248A -0.12997

235A -> 249A -0.10160

236A -> 238A -0.40323

237A -> 239A -0.35297

237A -> 241A -0.17487

231B -> 248B 0.12869

231B -> 249B -0.10172

232B -> 249B 0.10051

233B -> 237B 0.40190

234B -> 235B 0.42470

234B -> 240B -0.35126

Excited state symmetry could not be determined.

Excited State 9: 3.5607 eV 348.21 nm f=0.0658 <S\*\*2>=4.224

236A -> 239A -0.20267

236A -> 241A -0.10347

237A -> 238A -0.23598

216B -> 235B 0.13146

233B -> 235B 0.82444

233B -> 240B 0.24223

234B -> 237B -0.20855

Excited state symmetry could not be determined.

Excited State 10: 3.6123 eV 343.22 nm f=0.0002 <S\*\*2>=4.116

236A -> 238A 0.19182

237A -> 239A 0.16812

215B -> 235B -0.17587

218B -> 235B -0.18954

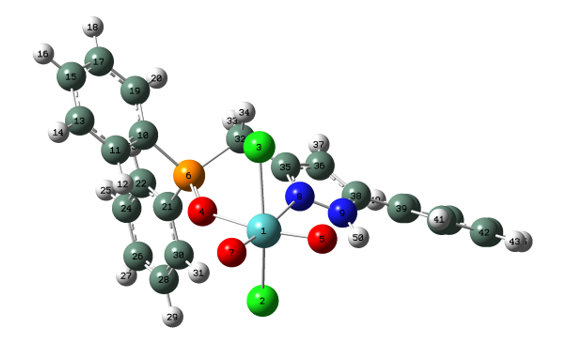
222B -> 235B 0.11160

224B -> 235B -0.13338

233B -> 237B -0.18662

234B -> 235B 0.79749

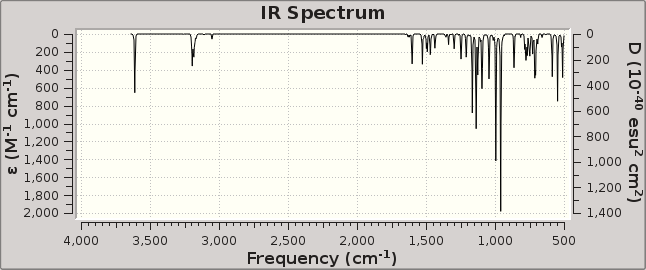
234B -> 240B 0.20793

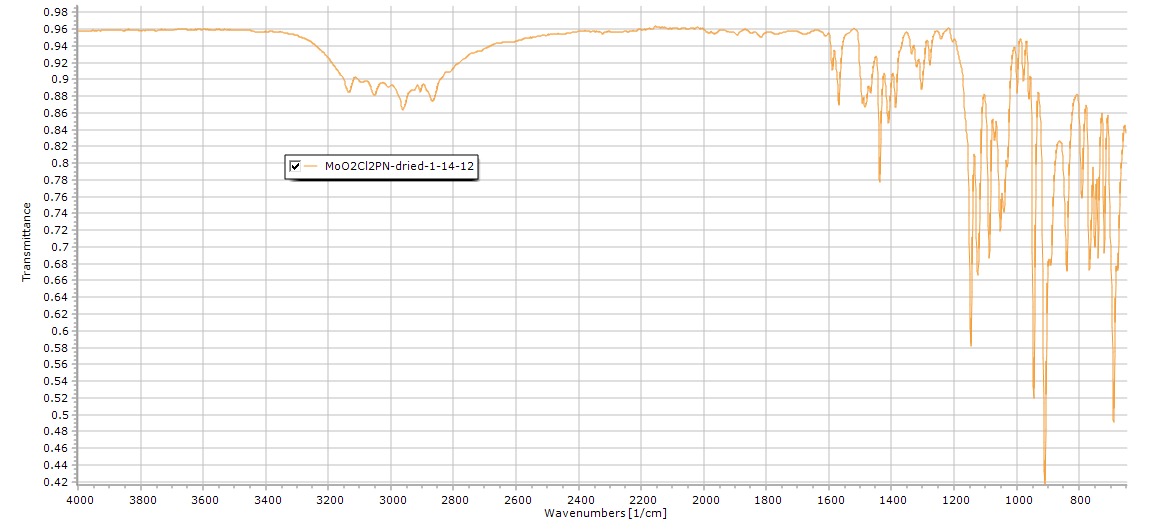


## **Figure S12**. Drawing of complex **3-THF** with atoms represented as spheres of arbitrary size (H-white, C-grey, N-blue and O-red) using the GaussView [1] program.

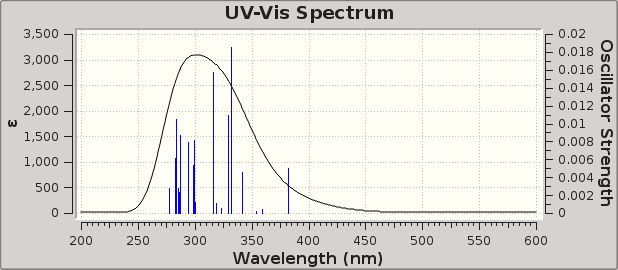
## **Table S3**. Atomic coordinates for 3-THF.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Row** | **Symbol** | **X** | **Y** | **Z** |
| 1 | Mo | 0.086855 | -2.30858 | 0.749534 |
| 2 | Cl | -0.77129 | -1.06986 | 2.660818 |
| 3 | Cl | 0.971937 | -2.65984 | -1.48426 |
| 4 | O | 1.476902 | -0.57469 | 0.69014 |
| 5 | O | -1.36859 | -3.19089 | 0.536603 |
| 6 | P | 1.781997 | 0.63781 | -0.1834 |
| 7 | O | 1.130298 | -3.37055 | 1.578721 |
| 8 | N | -1.15585 | -0.55977 | -0.4446 |
| 9 | N | -2.4906 | -0.54362 | -0.31526 |
| 10 | C | 3.426765 | 0.493876 | -0.93756 |
| 11 | C | 4.338673 | -0.37616 | -0.32931 |
| 12 | H | 4.033419 | -0.95171 | 0.536218 |
| 13 | C | 5.620017 | -0.51439 | -0.85613 |
| 14 | H | 6.321668 | -1.19413 | -0.38702 |
| 15 | C | 5.993871 | 0.206246 | -1.98897 |
| 16 | H | 6.990652 | 0.091935 | -2.39944 |
| 17 | C | 5.083847 | 1.065308 | -2.60355 |
| 18 | H | 5.368842 | 1.615338 | -3.49295 |
| 19 | C | 3.800717 | 1.209403 | -2.08193 |
| 20 | H | 3.099119 | 1.868075 | -2.58196 |
| 21 | C | 1.711533 | 2.153055 | 0.818682 |
| 22 | C | 2.291672 | 3.353573 | 0.387931 |
| 23 | H | 2.842074 | 3.399855 | -0.54497 |
| 24 | C | 2.185316 | 4.49725 | 1.17351 |
| 25 | H | 2.640074 | 5.423406 | 0.841189 |
| 26 | C | 1.506905 | 4.446295 | 2.391865 |
| 27 | H | 1.430113 | 5.337354 | 3.004791 |
| 28 | C | 0.937251 | 3.25125 | 2.824644 |
| 29 | H | 0.41661 | 3.207104 | 3.774244 |
| 30 | C | 1.036863 | 2.100867 | 2.043656 |
| 31 | H | 0.601837 | 1.167419 | 2.380784 |
| 32 | C | 0.568747 | 0.803422 | -1.56353 |
| 33 | H | 0.652718 | 1.802773 | -1.99488 |
| 34 | H | 0.871544 | 0.067799 | -2.31414 |
| 35 | C | -0.84245 | 0.540717 | -1.13383 |
| 36 | C | -2.00426 | 1.278845 | -1.42361 |
| 37 | H | -2.07454 | 2.192261 | -1.99057 |
| 38 | C | -3.05887 | 0.54873 | -0.88138 |
| 39 | C | -4.50553 | 0.786606 | -0.87866 |
| 40 | C | -5.41462 | -0.28136 | -0.85299 |
| 41 | H | -5.05418 | -1.30405 | -0.86649 |
| 42 | C | -6.78535 | -0.04144 | -0.84558 |
| 43 | H | -7.47513 | -0.87728 | -0.82832 |
| 44 | C | -7.26955 | 1.265251 | -0.87302 |
| 45 | H | -8.33746 | 1.450271 | -0.86976 |
| 46 | C | -6.37328 | 2.333077 | -0.90622 |
| 47 | H | -6.74268 | 3.35207 | -0.92253 |
| 48 | C | -5.00246 | 2.097529 | -0.90515 |
| 49 | H | -4.31124 | 2.932288 | -0.9047 |
| 50 | H | -2.92089 | -1.27791 | 0.23152 |





## **Figure S13**. Uncorrected calculated FTIR (top) and experimental (neat) spectrum of compound **3-THF**.



## **Figure S14**. Calculated UV-Vis spectrum for **3-THF**.

## **Table S4**. Excitation Energies and Oscillator Strengths for **3-THF**.

Excited State 1: Singlet-A 3.2471 eV 381.84 nm f=0.0050 <S\*\*2>=0.000

123 ->127 0.12167

124 ->127 -0.16728

125 ->127 0.16951

126 ->127 0.63847

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -2513.41919938

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.4514 eV 359.23 nm f=0.0004 <S\*\*2>=0.000

125 ->127 0.64720

125 ->128 -0.12494

126 ->127 -0.17906

Excited State 3: Singlet-A 3.5023 eV 354.01 nm f=0.0002 <S\*\*2>=0.000

115 ->127 -0.32597

117 ->127 0.28114

118 ->127 -0.12711

120 ->127 0.12828

122 ->127 0.24040

123 ->127 0.32876

124 ->127 0.30449

Excited State 4: Singlet-A 3.6306 eV 341.50 nm f=0.0046 <S\*\*2>=0.000

115 ->127 0.13256

121 ->127 -0.17799

123 ->127 -0.33523

124 ->127 0.49530

126 ->127 0.19683

Excited State 5: Singlet-A 3.7328 eV 332.15 nm f=0.0186 <S\*\*2>=0.000

115 ->128 0.10084

120 ->127 0.12487

124 ->127 0.10330

126 ->128 0.63474

Excited State 6: Singlet-A 3.7609 eV 329.67 nm f=0.0110 <S\*\*2>=0.000

115 ->127 0.24921

120 ->127 0.41889

121 ->127 0.37316

125 ->128 0.11490

126 ->128 -0.14380

Excited State 7: Singlet-A 3.8384 eV 323.01 nm f=0.0006 <S\*\*2>=0.000

115 ->127 0.43593

115 ->128 0.25707

117 ->128 -0.15314

122 ->127 0.13802

122 ->128 -0.11521

123 ->127 0.27149

123 ->128 -0.17953

124 ->128 -0.11762

Excited State 8: Singlet-A 3.8950 eV 318.32 nm f=0.0011 <S\*\*2>=0.000

115 ->127 -0.17057

115 ->128 0.18463

123 ->127 -0.10403

123 ->128 -0.20541

125 ->128 0.57423

Excited State 9: Singlet-A 3.9266 eV 315.75 nm f=0.0157 <S\*\*2>=0.000

115 ->127 -0.19034

115 ->128 0.36534

117 ->128 -0.17443

120 ->127 0.18451

121 ->127 0.16534

123 ->127 -0.15981

123 ->128 -0.13077

124 ->128 -0.11009

125 ->128 -0.29745

126 ->128 -0.11307

Excited State 10: Singlet-A 4.1260 eV 300.49 nm f=0.0012 <S\*\*2>=0.000

116 ->127 -0.19279

117 ->127 0.41534

119 ->127 0.20407

120 ->127 0.27589

121 ->127 -0.18972

123 ->127 -0.17126

124 ->127 -0.25896

Excited State 11: Singlet-A 4.1473 eV 298.95 nm f=0.0082 <S\*\*2>=0.000

114 ->127 -0.10820

119 ->128 -0.12282

120 ->128 0.43022

121 ->128 0.27652

123 ->128 -0.23999

124 ->128 0.27854

Excited State 12: Singlet-A 4.1569 eV 298.26 nm f=0.0054 <S\*\*2>=0.000

114 ->127 -0.21378

116 ->127 0.11526

120 ->128 -0.18988

121 ->128 -0.35946

123 ->128 -0.16387

124 ->128 0.40779

126 ->128 0.11369

Excited State 13: Singlet-A 4.2136 eV 294.24 nm f=0.0079 <S\*\*2>=0.000

123 ->129 0.13524

124 ->129 -0.14728

125 ->129 0.10231

126 ->129 0.64243

Excited State 14: Singlet-A 4.3175 eV 287.17 nm f=0.0087 <S\*\*2>=0.000

114 ->127 0.11022

115 ->128 0.38021

116 ->127 -0.10648

121 ->127 -0.17473

122 ->128 0.19209

123 ->128 0.29609

124 ->128 0.23612

125 ->129 -0.23803

Excited State 15: Singlet-A 4.3318 eV 286.22 nm f=0.0024 <S\*\*2>=0.000

114 ->127 -0.12438

116 ->127 0.11857

119 ->127 0.58812

121 ->127 0.18587

123 ->128 0.10847

Excited State 16: Singlet-A 4.3527 eV 284.84 nm f=0.0028 <S\*\*2>=0.000

117 ->127 -0.26979

118 ->127 0.14080

119 ->127 0.16146

120 ->127 0.27534

121 ->127 -0.34060

123 ->127 0.19035

125 ->129 0.34391

Excited State 17: Singlet-A 4.3664 eV 283.95 nm f=0.0033 <S\*\*2>=0.000

119 ->127 -0.10206

120 ->127 -0.22383

122 ->127 0.46846

123 ->127 -0.22261

125 ->129 0.34356

Excited State 18: Singlet-A 4.3727 eV 283.54 nm f=0.0105 <S\*\*2>=0.000

115 ->128 -0.13048

117 ->127 -0.24402

118 ->127 0.17097

122 ->127 0.39881

123 ->128 -0.17797

125 ->129 -0.36097

Excited State 19: Singlet-A 4.3880 eV 282.55 nm f=0.0061 <S\*\*2>=0.000

113 ->127 -0.11385

114 ->127 0.27748

116 ->127 -0.31403

118 ->127 0.32745

119 ->127 0.21072

120 ->127 -0.13321

121 ->127 0.19691

123 ->127 0.10987

123 ->128 -0.10029

124 ->128 0.12495

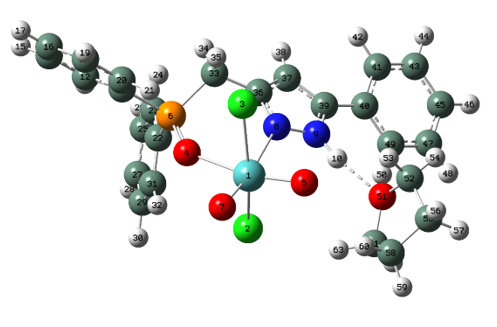
Excited State 20: Singlet-A 4.4726 eV 277.21 nm f=0.0028 <S\*\*2>=0.000

114 ->127 -0.21094

116 ->127 0.24946

117 ->127 0.24978

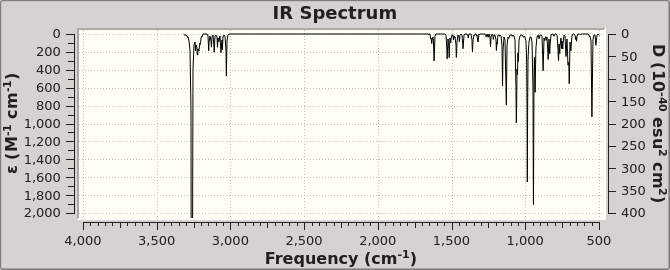
118 ->127 0.53318

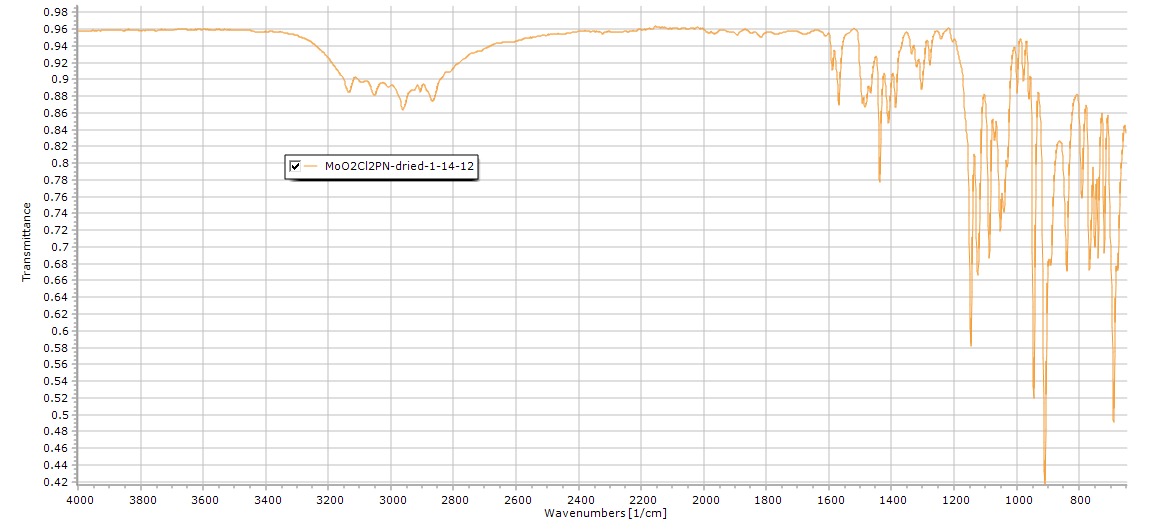
****

## **Figure S15**. Drawing of complex **3** with atoms represented as spheres of arbitrary size (H-white, C-grey, N-blue and O-red) using the GaussView [1] program.

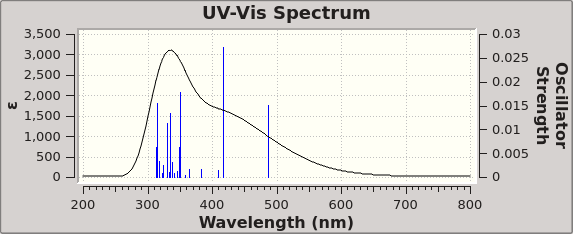
## **Table S5**. Atomic coordinates for **3**.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Row** | **Symbol** | **X** | **Y** | **Z** |
| 1 | Mo | 0.103201 | -2.11335 | 0.260193 |
| 2 | Cl | -0.43066 | -1.00032 | 2.349646 |
| 3 | Cl | 0.902324 | -2.36761 | -2.03236 |
| 4 | O | 1.944797 | -0.88518 | 0.442124 |
| 5 | O | -1.50865 | -2.58572 | -0.08158 |
| 6 | P | 2.534305 | 0.412901 | -0.10215 |
| 7 | O | 0.821416 | -3.51643 | 0.906753 |
| 8 | N | -0.60145 | 0.088514 | -0.63169 |
| 9 | N | -1.87649 | 0.510649 | -0.5193 |
| 10 | H | -2.59628 | -0.12392 | -0.14073 |
| 11 | C | 4.221174 | 0.125515 | -0.71609 |
| 12 | C | 5.271273 | 1.024325 | -0.49616 |
| 13 | H | 5.111051 | 1.926499 | 0.081444 |
| 14 | C | 6.539307 | 0.74925 | -1.00411 |
| 15 | H | 7.351608 | 1.444835 | -0.82721 |
| 16 | C | 6.764044 | -0.42156 | -1.72557 |
| 17 | H | 7.752778 | -0.63529 | -2.11569 |
| 18 | C | 5.721796 | -1.32381 | -1.93662 |
| 19 | H | 5.897458 | -2.24082 | -2.48698 |
| 20 | C | 4.45169 | -1.0575 | -1.43353 |
| 21 | H | 3.645726 | -1.76694 | -1.58396 |
| 22 | C | 2.567005 | 1.709308 | 1.167332 |
| 23 | C | 2.740337 | 3.0634 | 0.850313 |
| 24 | H | 2.84718 | 3.383698 | -0.18034 |
| 25 | C | 2.770062 | 4.017047 | 1.863842 |
| 26 | H | 2.900253 | 5.064101 | 1.615613 |
| 27 | C | 2.624316 | 3.624272 | 3.19442 |
| 28 | H | 2.643155 | 4.369007 | 3.982094 |
| 29 | C | 2.443068 | 2.279777 | 3.510954 |
| 30 | H | 2.313993 | 1.975275 | 4.54295 |
| 31 | C | 2.41317 | 1.319373 | 2.50226 |
| 32 | H | 2.243047 | 0.276727 | 2.73901 |
| 33 | C | 1.529979 | 1.003049 | -1.52123 |
| 34 | H | 1.910685 | 1.966097 | -1.86646 |
| 35 | H | 1.698218 | 0.268547 | -2.31448 |
| 36 | C | 0.071574 | 1.101046 | -1.1942 |
| 37 | C | -0.78696 | 2.18226 | -1.43409 |
| 38 | H | -0.52719 | 3.139664 | -1.85385 |
| 39 | C | -2.04189 | 1.771091 | -0.99092 |
| 40 | C | -3.31817 | 2.497826 | -0.99322 |
| 41 | C | -3.51317 | 3.546954 | -1.90531 |
| 42 | H | -2.738 | 3.783661 | -2.62469 |
| 43 | C | -4.69937 | 4.272815 | -1.91131 |
| 44 | H | -4.83288 | 5.077263 | -2.62578 |
| 45 | C | -5.71661 | 3.960674 | -1.01002 |
| 46 | H | -6.64221 | 4.524934 | -1.01508 |
| 47 | C | -5.53559 | 2.916159 | -0.10533 |
| 48 | H | -6.32076 | 2.665855 | 0.599162 |
| 49 | C | -4.34794 | 2.190066 | -0.09229 |
| 50 | H | -4.2271 | 1.378563 | 0.613091 |
| 51 | O | -4.09726 | -1.04951 | 0.382264 |
| 52 | C | -4.65038 | -1.85642 | -0.6859 |
| 53 | H | -3.82642 | -2.21206 | -1.31165 |
| 54 | H | -5.31145 | -1.22132 | -1.28004 |
| 55 | C | -5.36827 | -3.01779 | 0.000846 |
| 56 | H | -5.41181 | -3.90606 | -0.63204 |
| 57 | H | -6.39237 | -2.73526 | 0.264321 |
| 58 | C | -4.51869 | -3.21804 | 1.265388 |
| 59 | H | -5.05774 | -3.72262 | 2.069632 |
| 60 | H | -3.61982 | -3.79186 | 1.032319 |
| 61 | C | -4.14039 | -1.78407 | 1.634348 |
| 62 | H | -4.89874 | -1.31727 | 2.274187 |
| 63 | H | -3.16484 | -1.69923 | 2.113033 |

****



## **Figure S16**. Uncorrected calculated FTIR (top) and experimental (neat) spectrum of compound **3**.

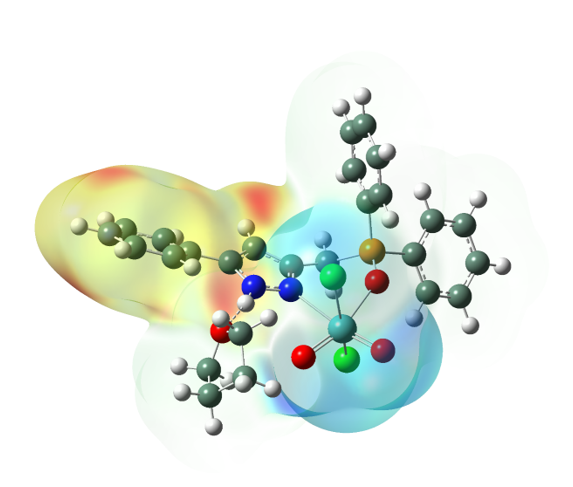
****

## **Figure S17**. Calculated UV-Vis spectrum for **3**.

## **Figure S18**. UV-vis absorption spectrum of **3** in CH2Cl2.

## **Figure S19**. Emission spectrum of **3** in CH2Cl2.

## **Figure S20**. Emission spectrum of solvent CH2Cl2.



## **Figure S21**. Difference density illustrations as iso-surfaces of complex **3** featuring excited state 1. Red areas indicate values for the different density of -1.630e-4 and blue are for 1.630e+4, see scale on top of illustration.

## **Table S6**. Excitation Energies and Oscillator Strengths for **3**.

Excited State 1: Singlet-A 2.5491 eV 486.38 nm f=0.0150 <S\*\*2>=0.000

146 ->147 0.69782

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -2745.81946723

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.9720 eV 417.18 nm f=0.0273 <S\*\*2>=0.000

146 ->148 0.69826

Excited State 3: Singlet-A 3.0269 eV 409.60 nm f=0.0014 <S\*\*2>=0.000

144 ->147 0.10857

145 ->147 0.68291

Excited State 4: Singlet-A 3.2438 eV 382.22 nm f=0.0016 <S\*\*2>=0.000

139 ->147 0.10870

143 ->147 0.57198

144 ->147 0.36299

Excited State 5: Singlet-A 3.3987 eV 364.80 nm f=0.0018 <S\*\*2>=0.000

138 ->147 0.43782

138 ->148 0.10518

139 ->147 -0.11074

140 ->147 0.10225

141 ->147 0.24170

142 ->147 0.18035

145 ->148 -0.39444

Excited State 6: Singlet-A 3.4649 eV 357.83 nm f=0.0003 <S\*\*2>=0.000

138 ->147 0.28953

141 ->147 0.17741

142 ->147 0.11876

145 ->147 0.14031

145 ->148 0.54863

Excited State 7: Singlet-A 3.5307 eV 351.16 nm f=0.0177 <S\*\*2>=0.000

143 ->147 -0.12292

144 ->147 0.20200

146 ->149 0.65613

Excited State 8: Singlet-A 3.5347 eV 350.76 nm f=0.0025 <S\*\*2>=0.000

143 ->147 -0.31811

144 ->147 0.54582

146 ->149 -0.23116

Excited State 9: Singlet-A 3.5599 eV 348.28 nm f=0.0062 <S\*\*2>=0.000

134 ->147 -0.25364

137 ->147 0.35126

138 ->147 -0.18130

139 ->147 0.16234

142 ->147 0.47008

Excited State 10: Singlet-A 3.5883 eV 345.52 nm f=0.0012 <S\*\*2>=0.000

130 ->147 -0.11303

131 ->147 0.25360

132 ->147 -0.25513

133 ->147 -0.18508

134 ->147 0.18465

135 ->147 0.35829

136 ->147 0.27870

139 ->147 0.12867

143 ->147 -0.13991

Excited State 11: Singlet-A 3.6339 eV 341.19 nm f=0.0008 <S\*\*2>=0.000

134 ->147 -0.15779

137 ->147 0.27830

141 ->147 0.43667

142 ->147 -0.41895

Excited State 12: Singlet-A 3.6619 eV 338.58 nm f=0.0031 <S\*\*2>=0.000

135 ->148 0.10235

136 ->147 -0.12966

137 ->147 0.11875

138 ->148 0.11659

140 ->147 -0.11182

143 ->148 0.52579

144 ->148 0.33012

Excited State 13: Singlet-A 3.6944 eV 335.60 nm f=0.0135 <S\*\*2>=0.000

135 ->147 -0.17235

136 ->147 0.26236

137 ->147 -0.21965

138 ->147 -0.30606

139 ->147 -0.10450

140 ->147 0.30958

141 ->147 0.25667

143 ->147 0.11266

143 ->148 0.14856

144 ->148 0.10547

Excited State 14: Singlet-A 3.7167 eV 333.59 nm f=0.0010 <S\*\*2>=0.000

137 ->147 0.19953

138 ->147 0.12748

140 ->147 0.52823

141 ->147 -0.33481

142 ->147 -0.14809

Excited State 15: Singlet-A 3.7512 eV 330.52 nm f=0.0113 <S\*\*2>=0.000

131 ->147 -0.20081

132 ->147 0.23213

133 ->147 0.11226

134 ->147 -0.12937

136 ->147 0.52577

138 ->147 0.12342

140 ->147 -0.14386

Excited State 16: Singlet-A 3.8175 eV 324.78 nm f=0.0025 <S\*\*2>=0.000

132 ->147 0.10794

137 ->147 -0.21114

139 ->147 0.60557

140 ->147 0.12864

Excited State 17: Singlet-A 3.8500 eV 322.03 nm f=0.0009 <S\*\*2>=0.000

134 ->148 -0.12562

137 ->148 0.18299

138 ->148 0.41386

140 ->148 0.12445

141 ->148 0.30993

142 ->148 0.27591

144 ->148 -0.11529

145 ->148 0.11033

Excited State 18: Singlet-A 3.8980 eV 318.07 nm f=0.0033 <S\*\*2>=0.000

131 ->148 0.20817

132 ->147 0.12888

132 ->148 -0.20030

133 ->148 -0.13580

134 ->148 0.14031

135 ->147 0.36139

135 ->148 0.19463

136 ->148 0.13848

139 ->147 -0.13754

140 ->147 0.17768

144 ->148 -0.18004

Excited State 19: Singlet-A 3.9421 eV 314.51 nm f=0.0155 <S\*\*2>=0.000

131 ->147 -0.17530

131 ->148 -0.20522

132 ->147 0.11042

132 ->148 0.14978

133 ->148 0.11496

134 ->148 -0.10728

135 ->147 0.33580

135 ->148 -0.15446

136 ->147 -0.13084

143 ->148 -0.13205

144 ->148 0.33881

Excited State 20: Singlet-A 3.9547 eV 313.51 nm f=0.0063 <S\*\*2>=0.000

131 ->147 0.10568

131 ->148 0.15468

132 ->148 -0.13121

133 ->148 -0.10736

135 ->147 -0.15277

142 ->148 0.13066

143 ->148 -0.35212

144 ->148 0.44168

## **References**

[1] GaussView, V. 6, R. Dennington, T.A. Keith, J.M. Millam, in, Semichem Inc. Shawnee Mission, KS, 2016.