

**Supporting Information for**

**Selenadiazolopyridine: A synthon for  
supramolecular assembly and complexes with  
metallophilic interactions**

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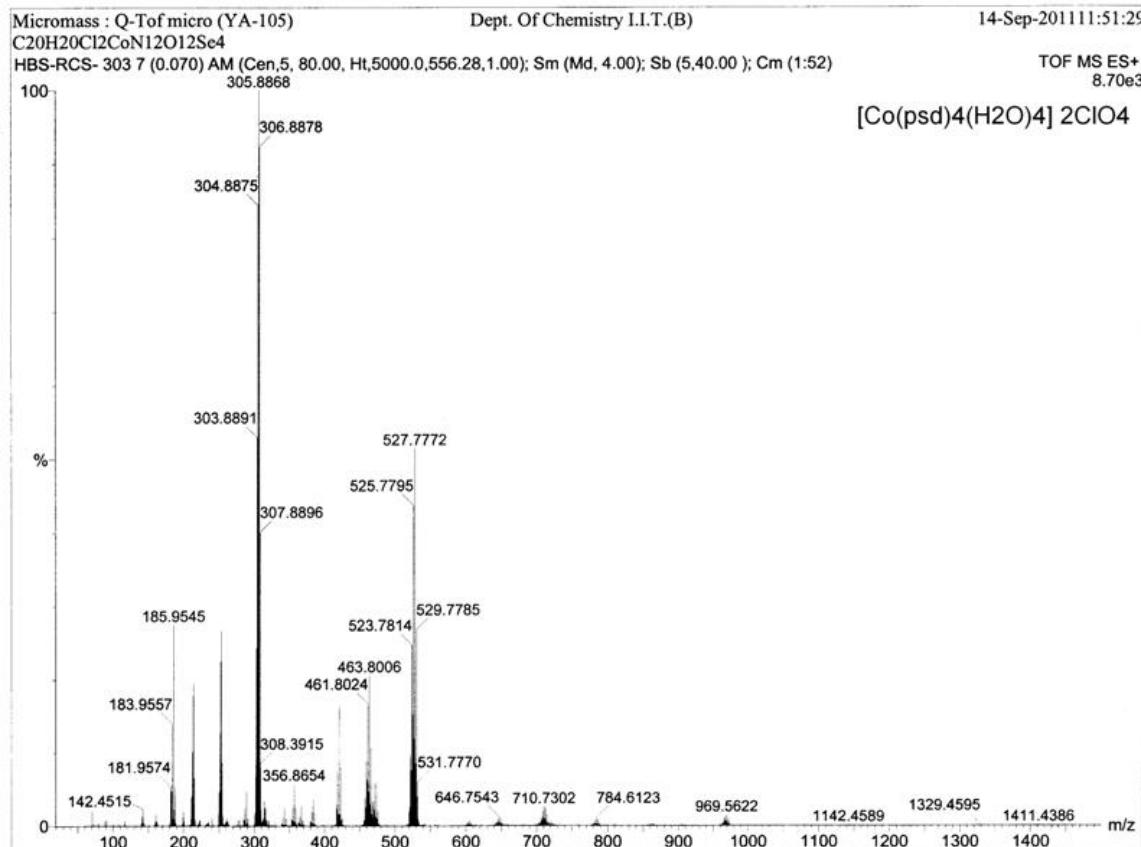
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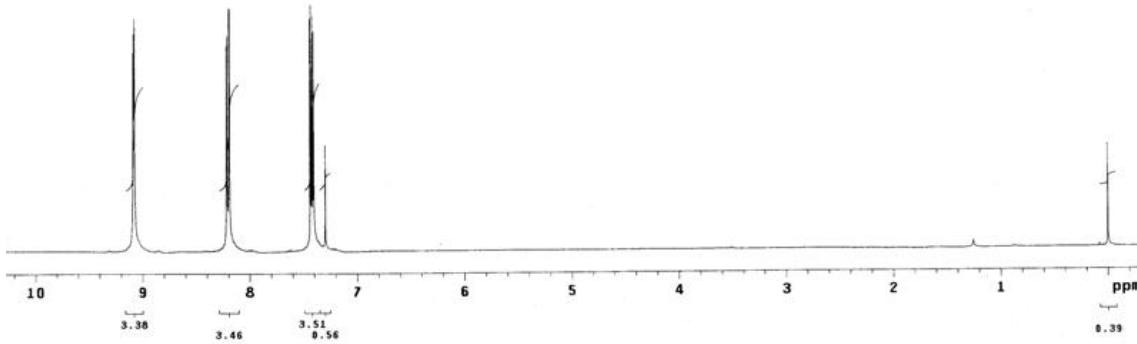
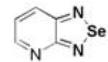
### Figure S1. ESI spectrum of 14.

```

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exp4 PROTON

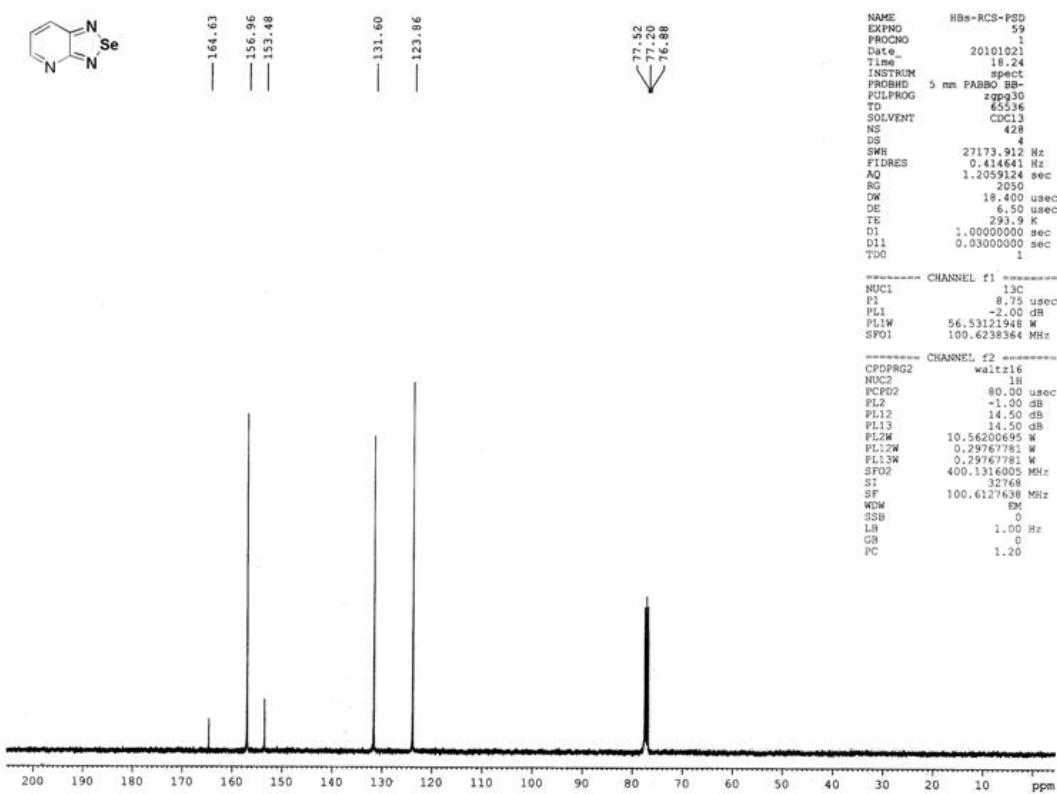
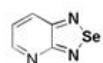
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solvent    CDCl3 gain    not used
file      exp spin   not used
ACQUISITION   1st    0.000
sw       18018.8 pw80   2.500
at        1.395 alfa   20.000
np        39962   FLAGS
fb      not used 11      n
bs        4   in      n
di        0   dp      y
nt       400   hs      nn
ct        56   PROCESSING
TRANSMITTER   H1      not used
tn          H1      DISPLAY
sfrq     399.883 sp     -139.0
tof      200.0   wp     4301.0
tpwr      55   rf1    2743.3
pw       4.250   fp      0
pw1      DECOUPLER   rp     41.6
dn        C13   lp     -138.4
dof       0   PLOT
ds       nme   wc     250
dm       c   sc      0
dpvr     51   vs     53
dmf     17100   th      4
nm      ph

```



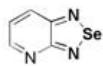
**Figure S2.** <sup>1</sup>H NMR spectrum of **5** in CDCl<sub>3</sub>.

HBS-RCS-PSD



**Figure S3.**  $^{13}\text{C}$  NMR spectrum of **5** in  $\text{CDCl}_3$ .

HBs-RCS-PSD

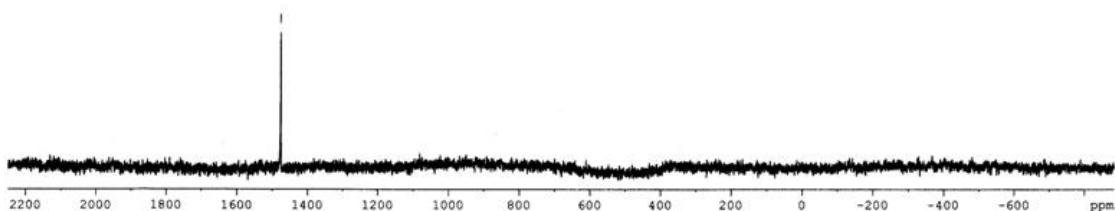


1476.095

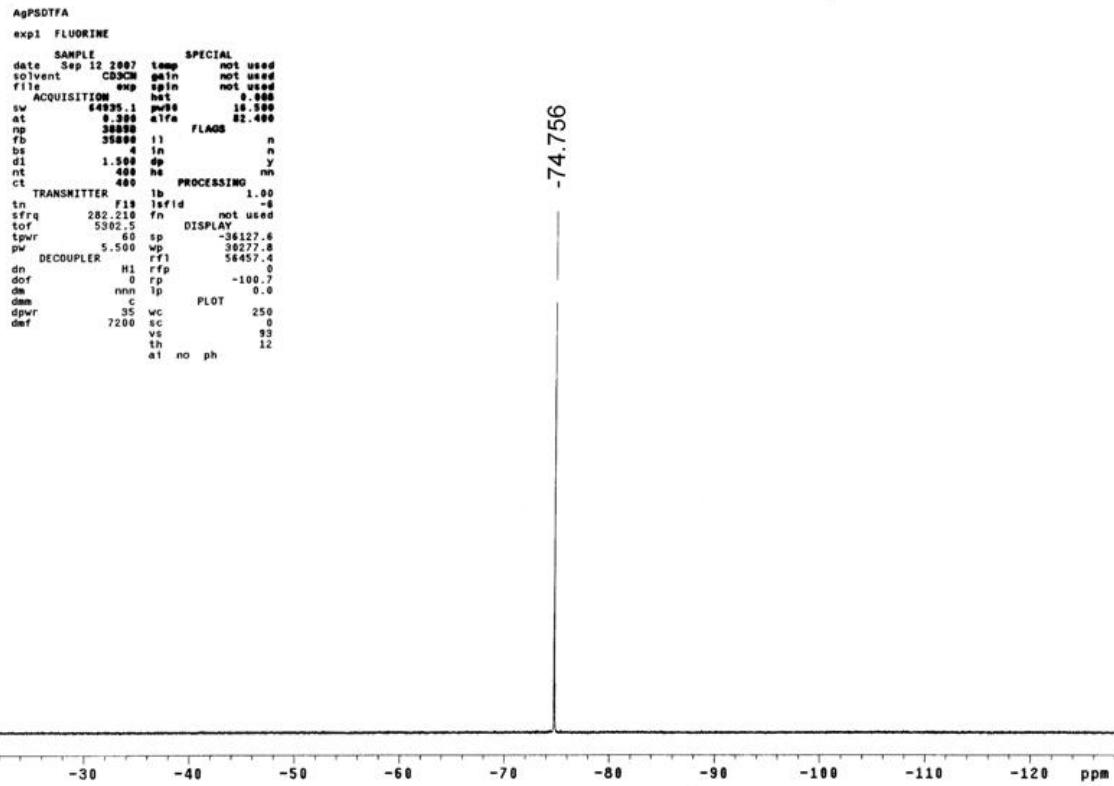
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EXPNO 58  
PROCNO 1  
Date 20101021  
Time 18.12  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg  
TD 65536  
SOLVENT CDCl3  
NS 500  
DS 4  
SWH 267857.156 Hz  
FIDRES 4.087176 Hz  
AQ 0.1223839 sec  
RG 228  
DW 1.867 usec  
DE 6.50 usec  
TE 294.0 K  
D1 1.0000000 sec  
TDO 1

===== CHANNEL f1 ======

NUC1 77Se  
P1 10.00 usec  
PL1 0.00 dB  
SFO1 76.3490004 MHz  
SI 65536  
SF 76.3110246 MHz  
WDW EM  
SSB 0  
LB 30.00 Hz  
GB 0  
PC 0.10



**Figure S4.** <sup>77</sup>Se NMR spectrum of **5** in CDCl<sub>3</sub>.



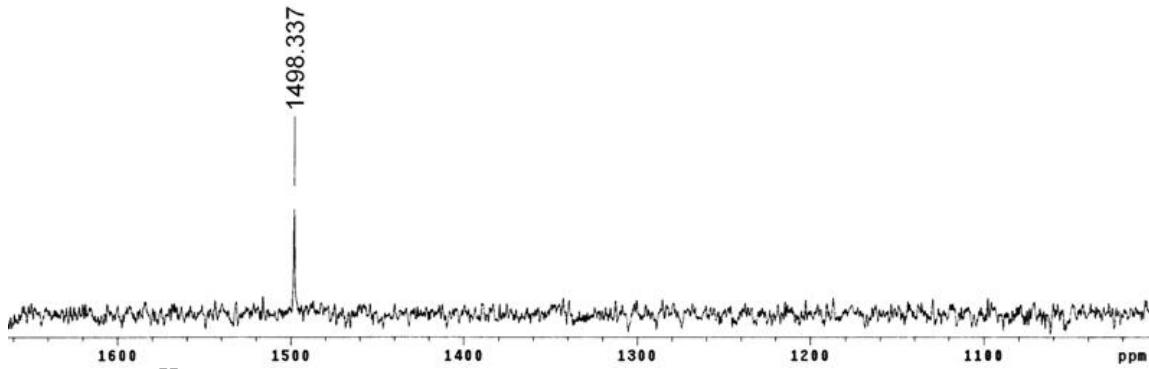
**Figure S5.**  $^{19}\text{F}$  NMR Spectrum of **10** in  $\text{CD}_3\text{CN}$ .

```

HBS-GM-AQPSD
Poor Solubility
Scanned for 2 hours
exp7 s2pul

SAMPLE           DEC. & VT
date  Feb 20 2007 dn   H1
solvent  DMSO dof   0
file    exp dm   nnn
        ACQUISITION dm   c
sfreq  57.308 dmf  200
tr    1.0000000000000002
at    0.640 1b   30.00
np    128000  fm   not used
sw    1000000.0
fb    55000.0 werr
bs    2 wexp
pw    3.0 wbs
pw1   3.0 wnt
tpwr  58 DISPLAY
d1    0 sp   57368.6
t0f   80000.0 wp   37502.8
nt    64000 vs   30924
ct    13794 sc   0
alock n wc   250
gain  6 hzmn 151.1
FLAGS  ls   837641.33
i1    n rrf1 -45726.2
in    n rfp  0
dp    y th   7
        ins  65.734
        ai cdc ph

```

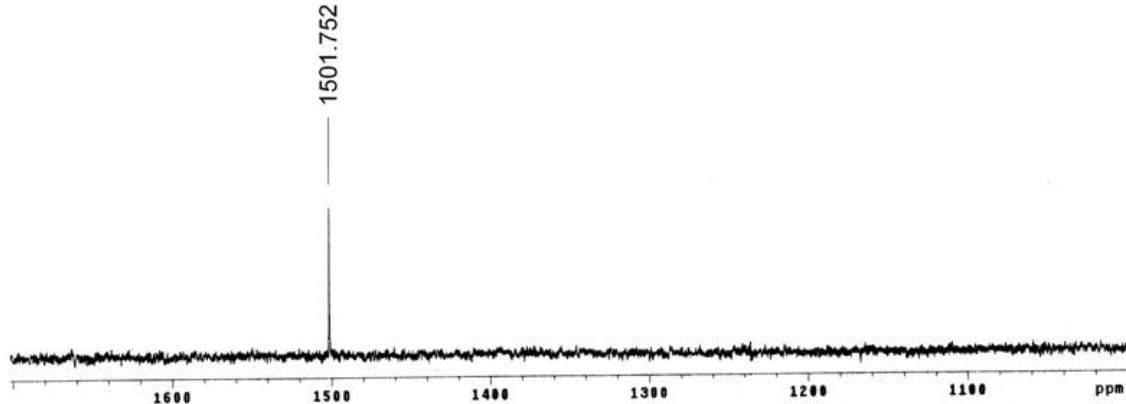


**Figure S6.**  $^{77}\text{Se}$  NMR spectrum of **9** in  $\text{DMSO-d}_6$ .

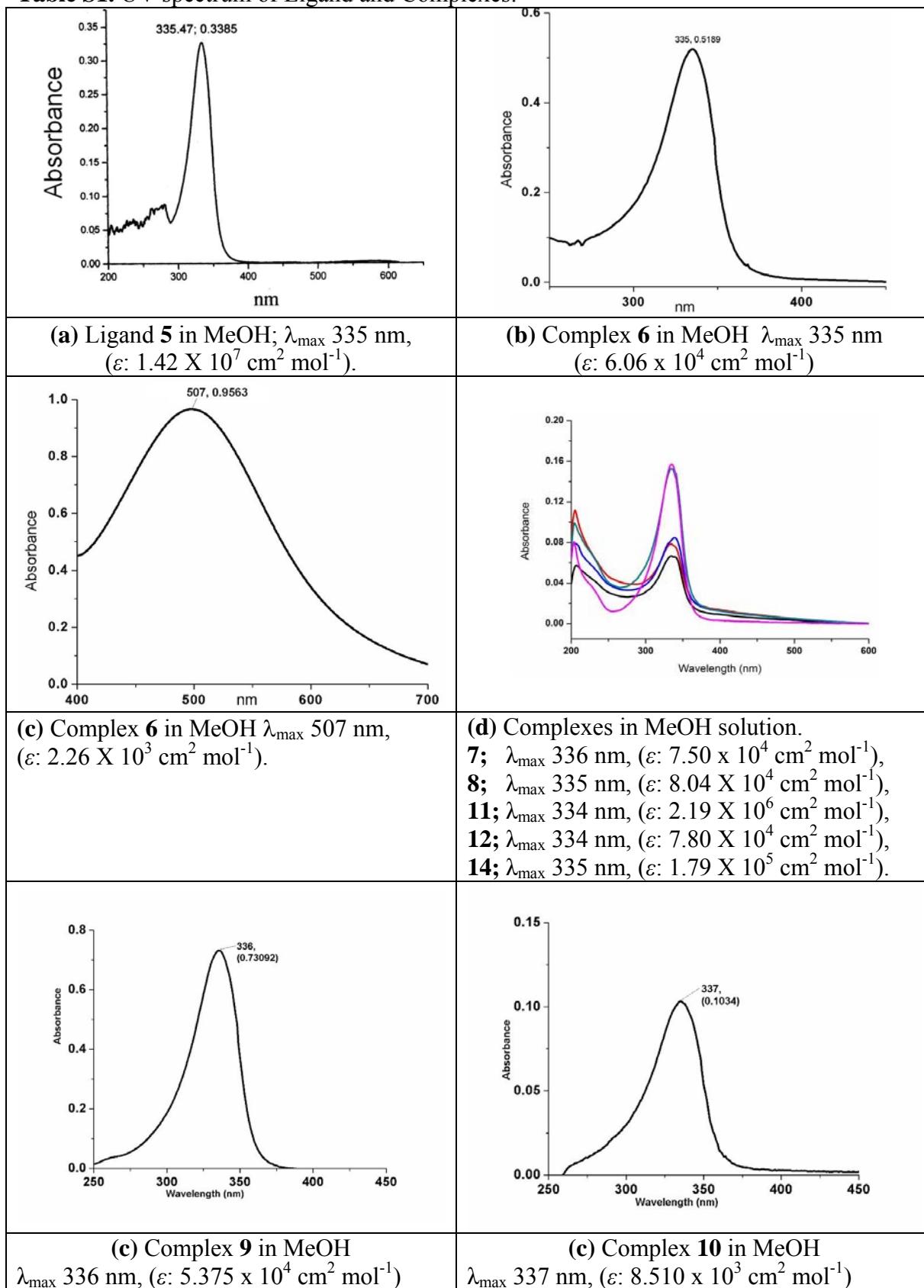
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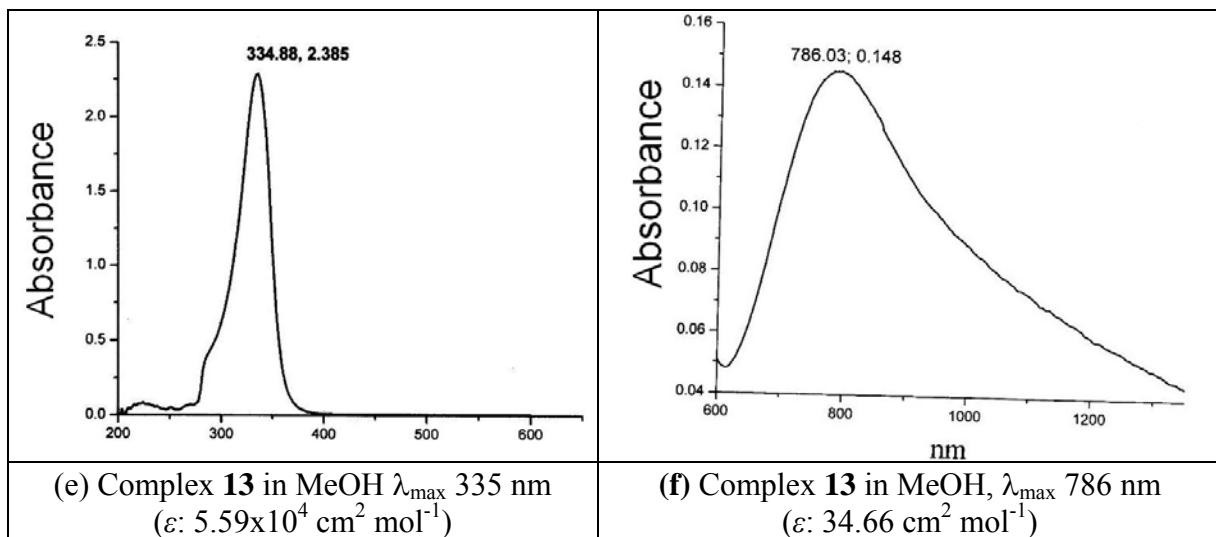
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solvent  DMSO dcf   0
file    exp dm   nnn
        ACQUISITION dm   c
sfreq  57.275 dmf  200
tr    1.0000000000000002
at    0.640 1b   10.00
np    128000 fm   not used
sw    1000000.0
fb    55000.0 werr
bs    2 wexp
pw    3.0 wbs
pw1   3.0 wnt
tpwr  58 DISPLAY
d1    0 sp   57158.0
t0f   55000.0 wp   40199.3
nt    64000 vs   5195
ct    568 sc   0
alock n wc   250
gain  6 hzmn 160.80
FLAGS  ls   837641.33
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in    n rfp  0
dp    y th   7
        ins  65.734
        ai cdc ph

```

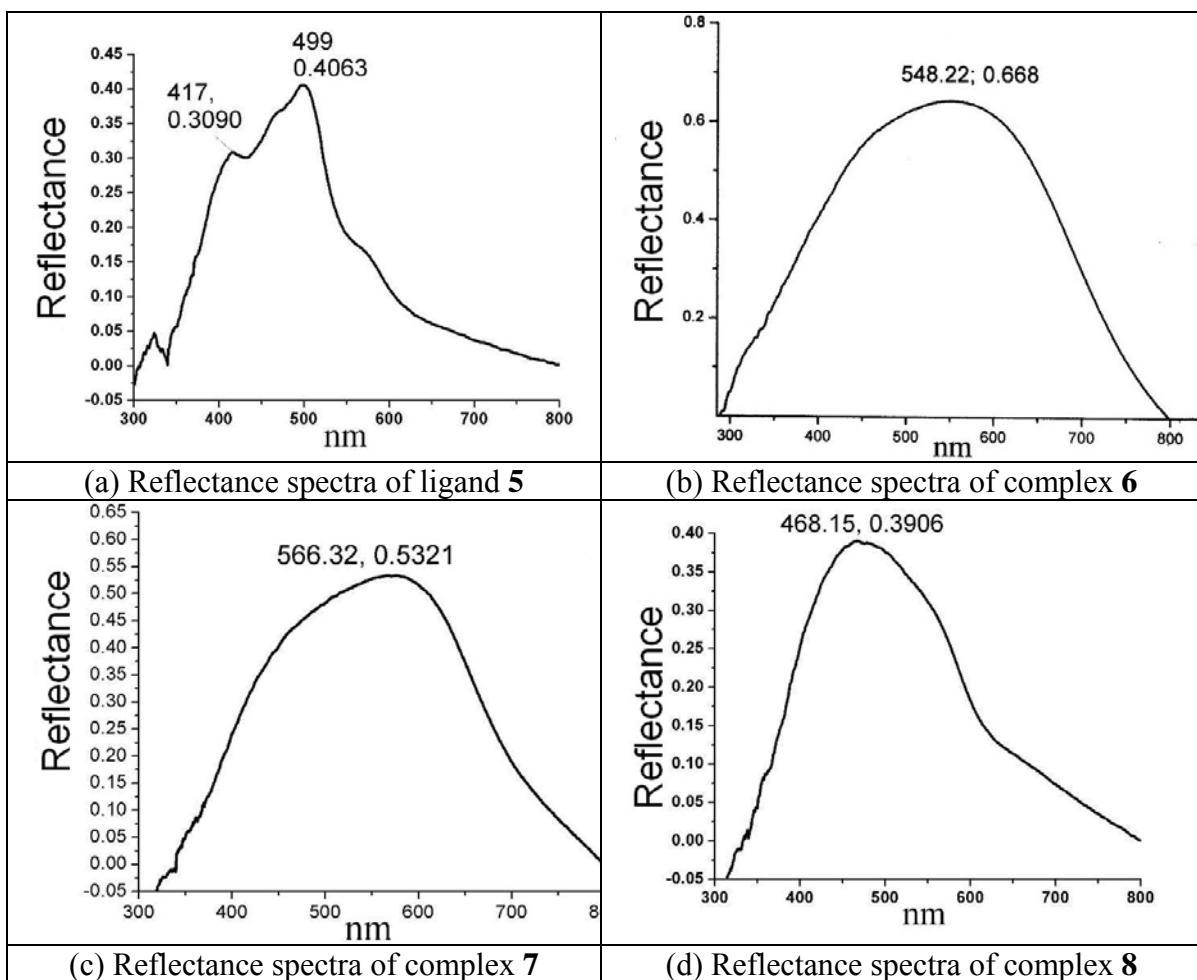


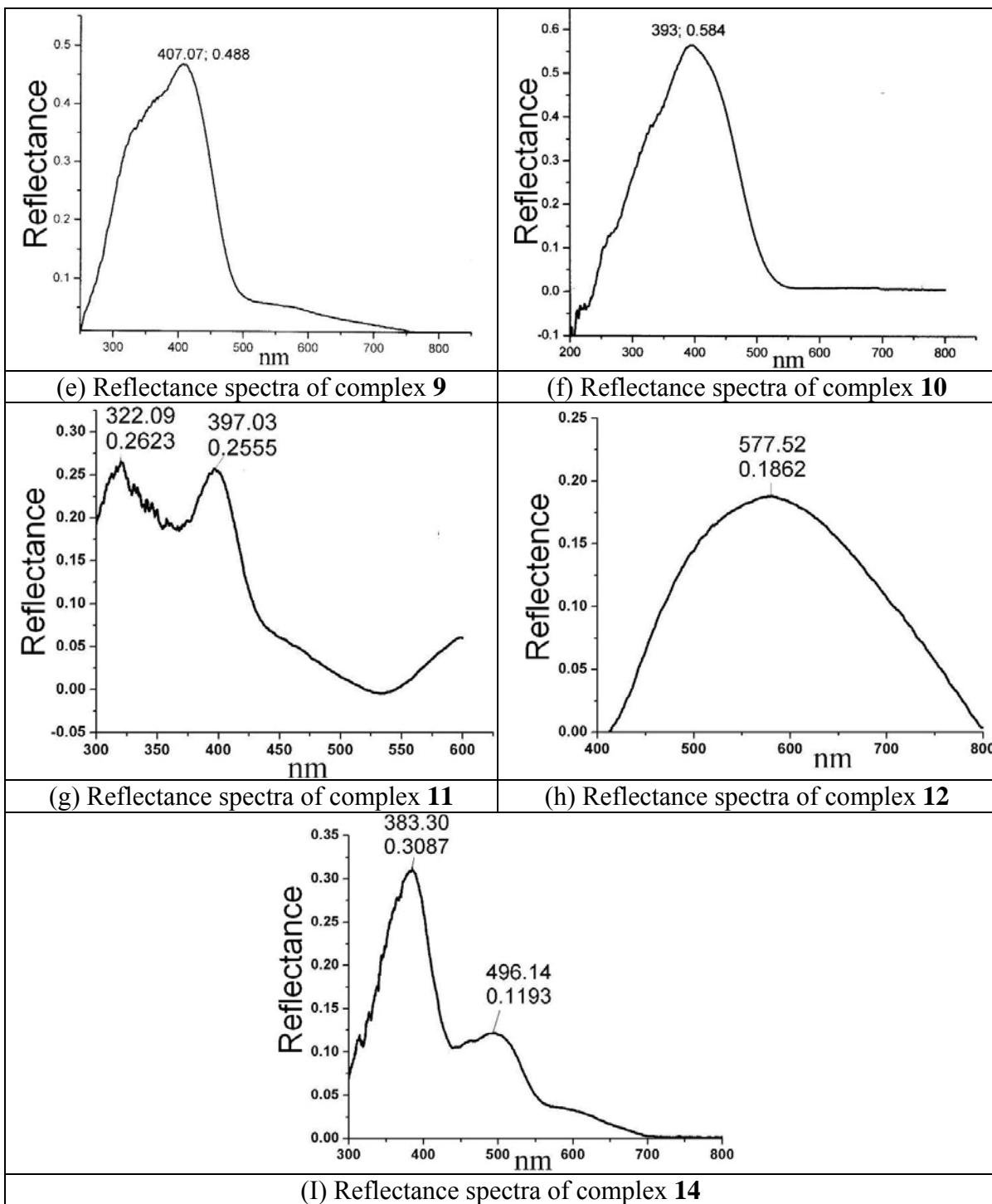
**Figure S7.**  $^{77}\text{Se}$  NMR spectrum of **10** in  $\text{DMSO-d}_6$ .

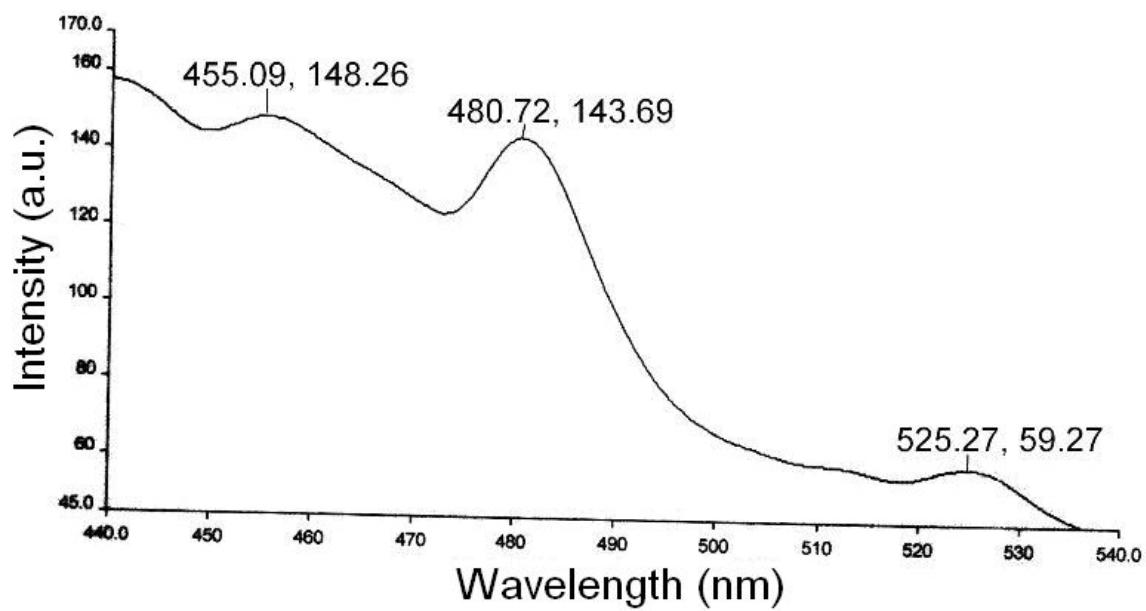
**Table S1.** UV spectrum of Ligand and Complexes:



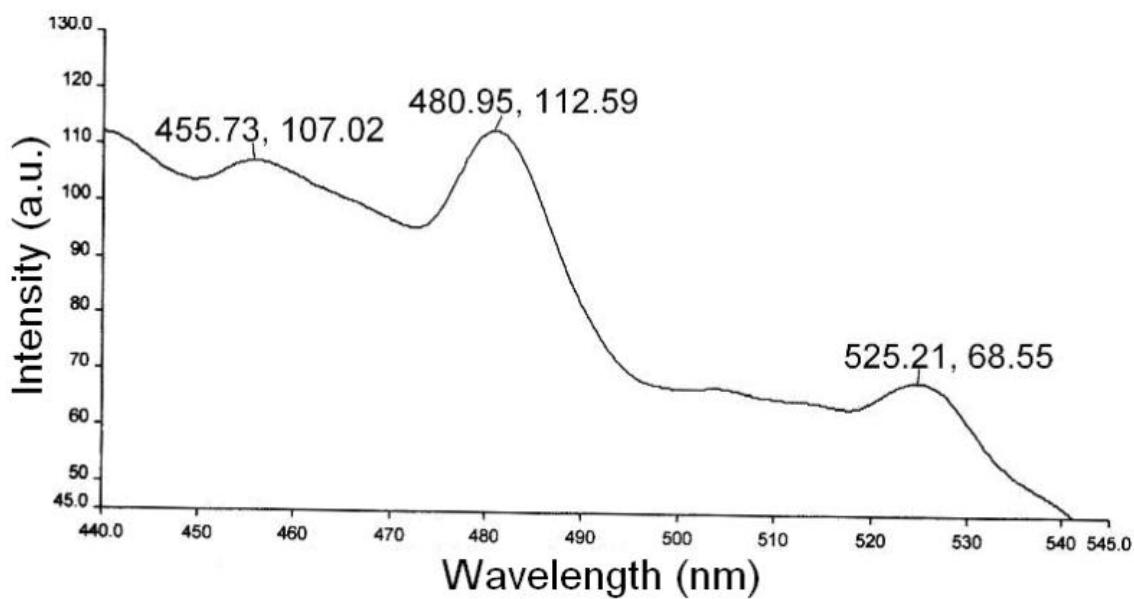
**Table S2.** Reflectance spectrum of ligand and Complexes .



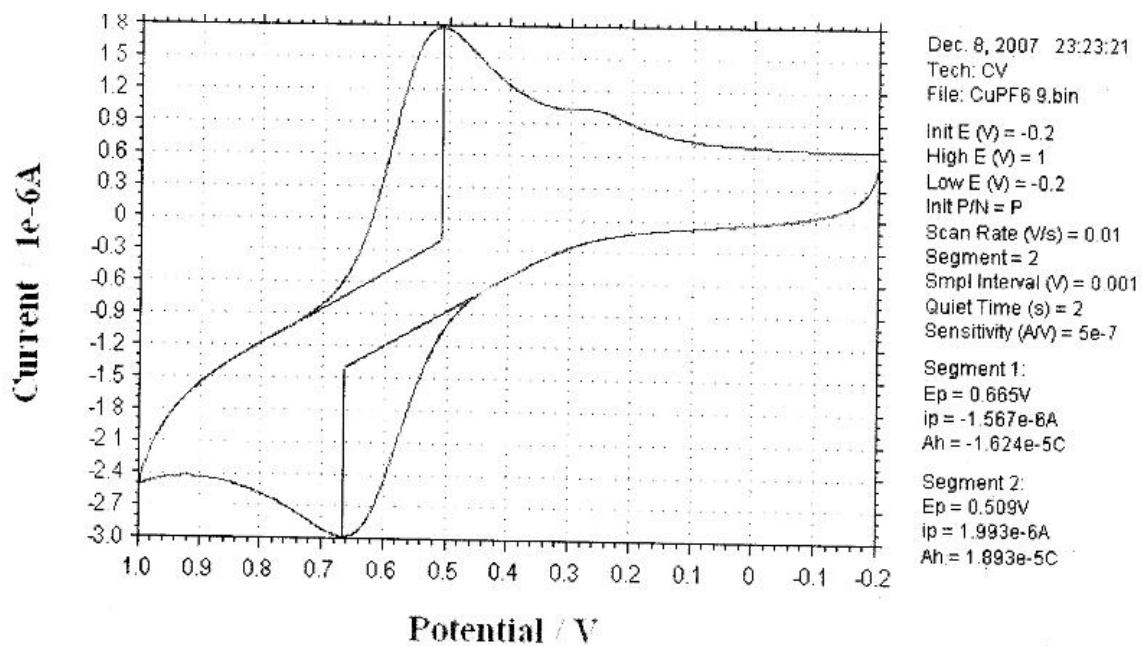




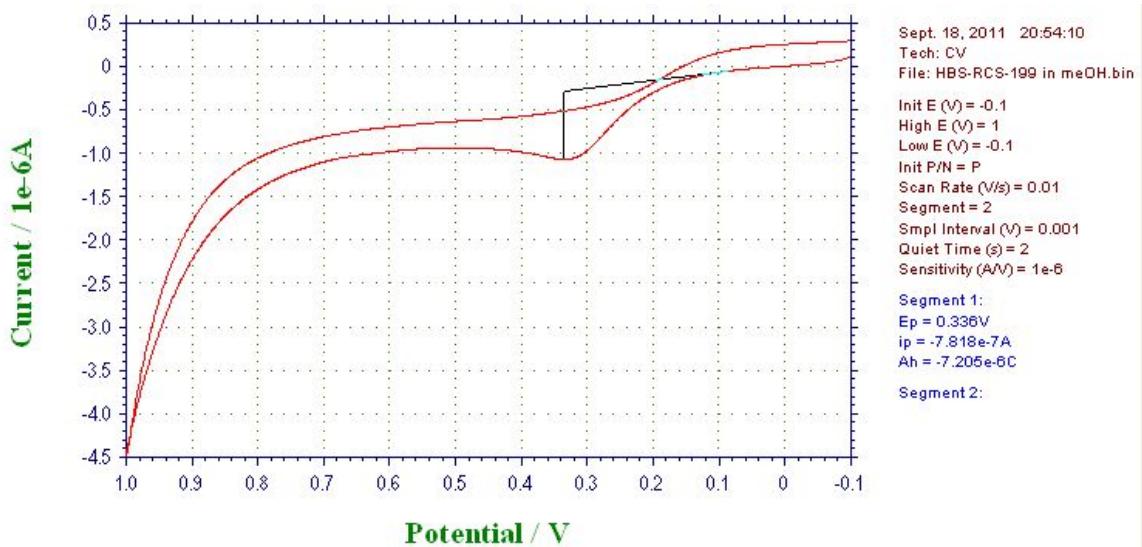
**Figure S8.** Emission Spectra of Complexes **9**.



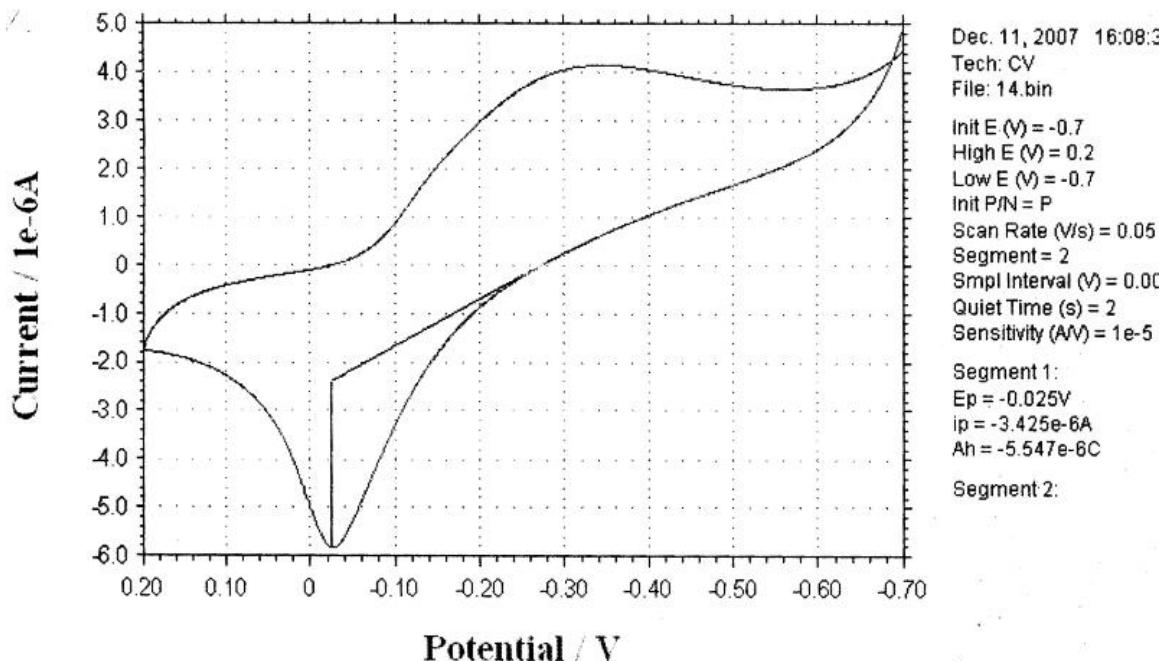
**Figure S9.** Emission Spectra of Complexes **10**.



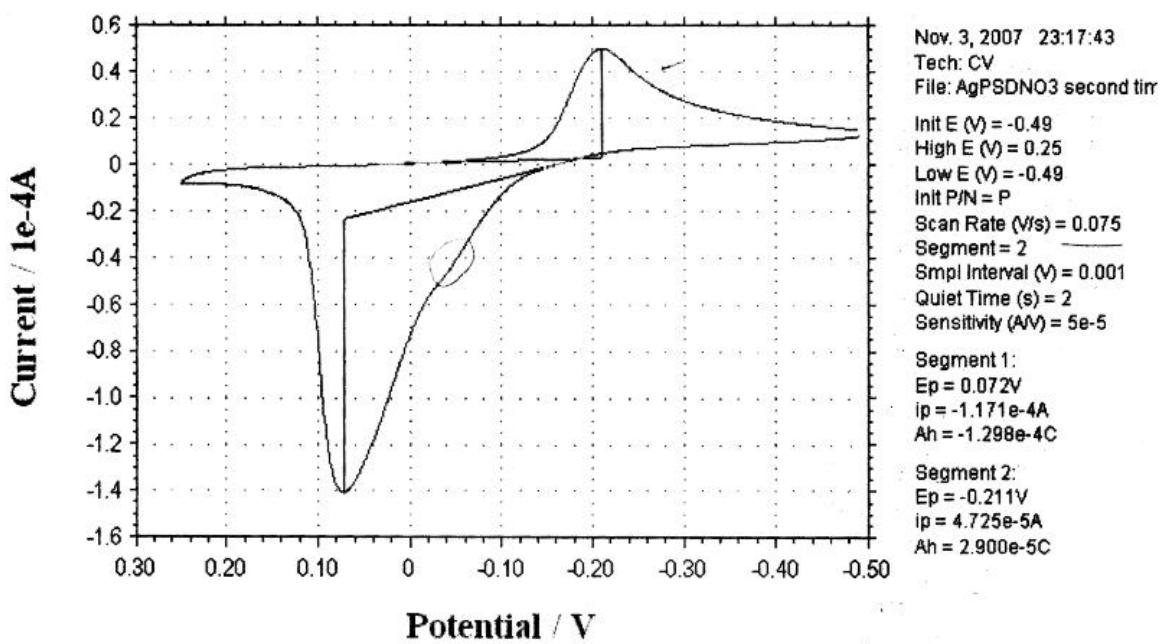
**Figure S10.** Cyclic Voltammogram of 6.



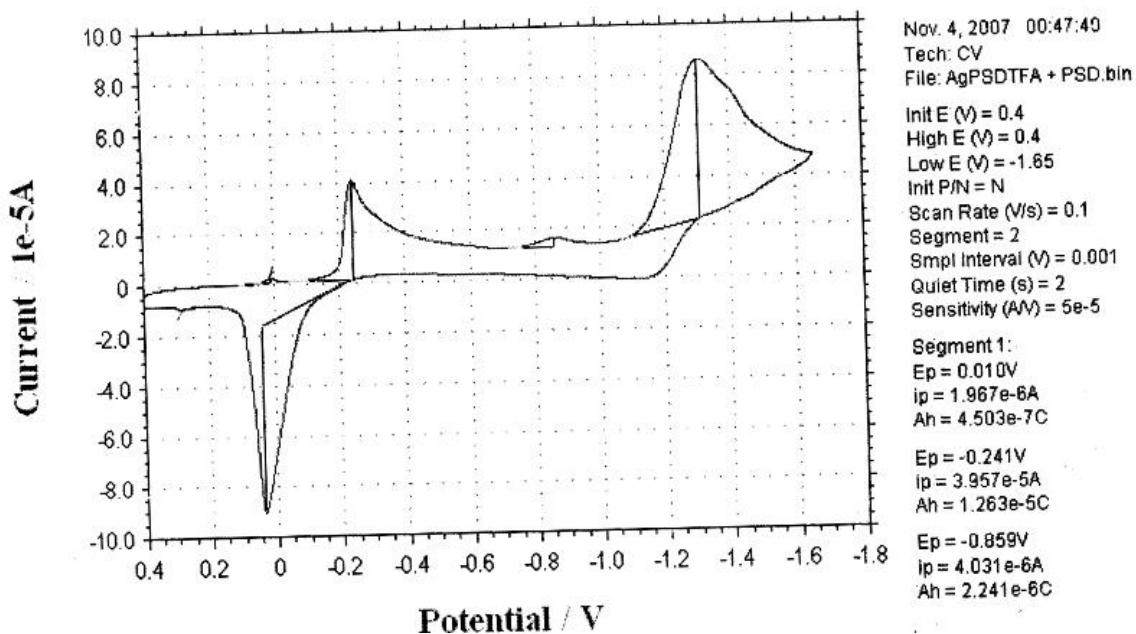
**Figure S11.** Cyclic Voltammogram of 8.



**Figure S12.** Cyclic Voltammogram of 13.



**Figure S13.** Cyclic Voltammogram of 9.



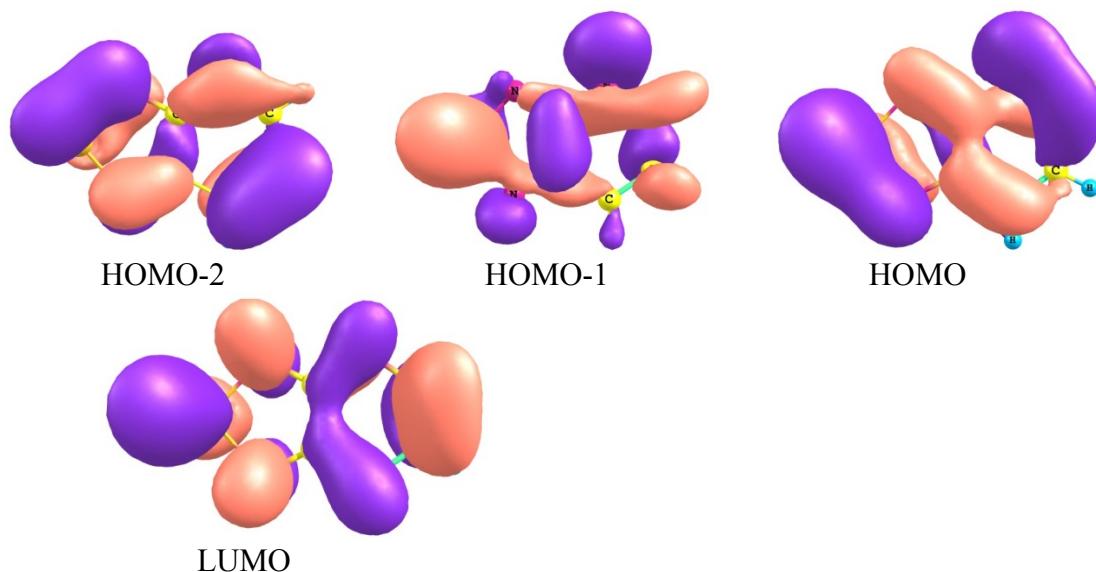
**Figure S14.** Cyclic Voltammogram of **10**.

#### Representative examples of TD-DFT (B3LYP/6-31G(d)) analysis:

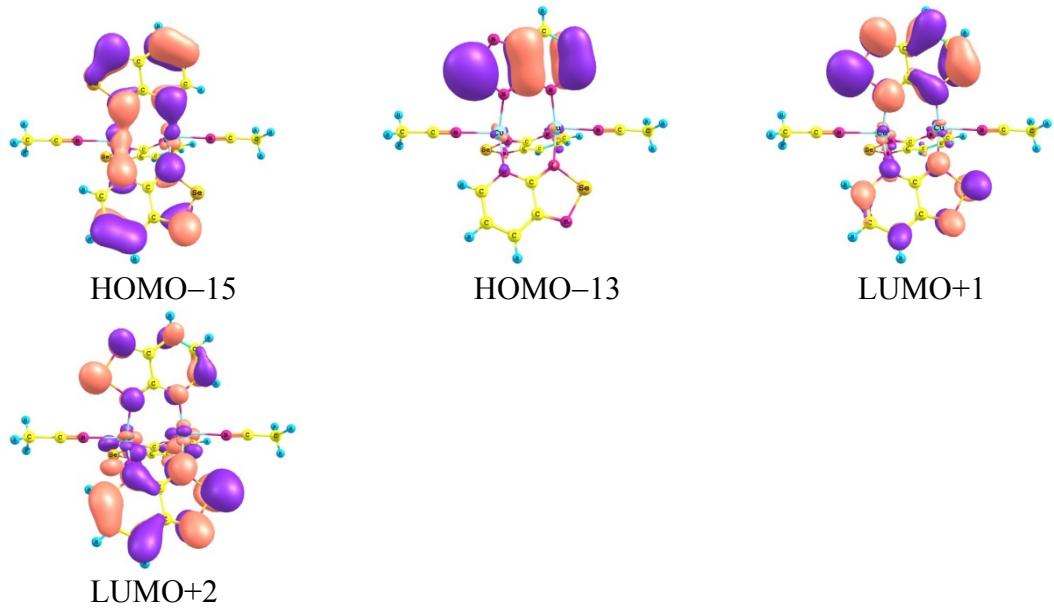
**Compound 5:**  $\lambda = 288 \text{ nm}$  ( $f = 0.234$ );

The major contributing MO's are as follows

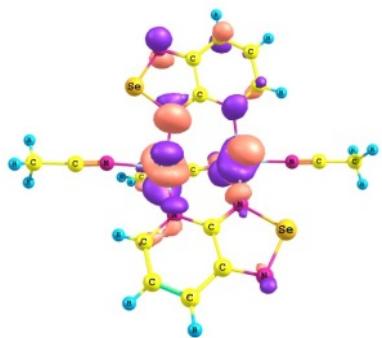
HOMO-2  $\rightarrow$  LUMO ; HOMO-1  $\rightarrow$  LUMO ; HOMO  $\rightarrow$  LUMO



**Compound 6:**  $\lambda = 296$  nm ( $f = 0.138$ );  $549$  nm ( $f = 0.040$ ),  
For transition at 296 nm, the major contributing MO's are shown below:  
HOMO-15→LUMO+2; HOMO-13→LUMO+1



For transition at 547 nm, the major contributing MO's are:  
HOMO-3→LUMO+1 ; HOMO-3→LUMO+2

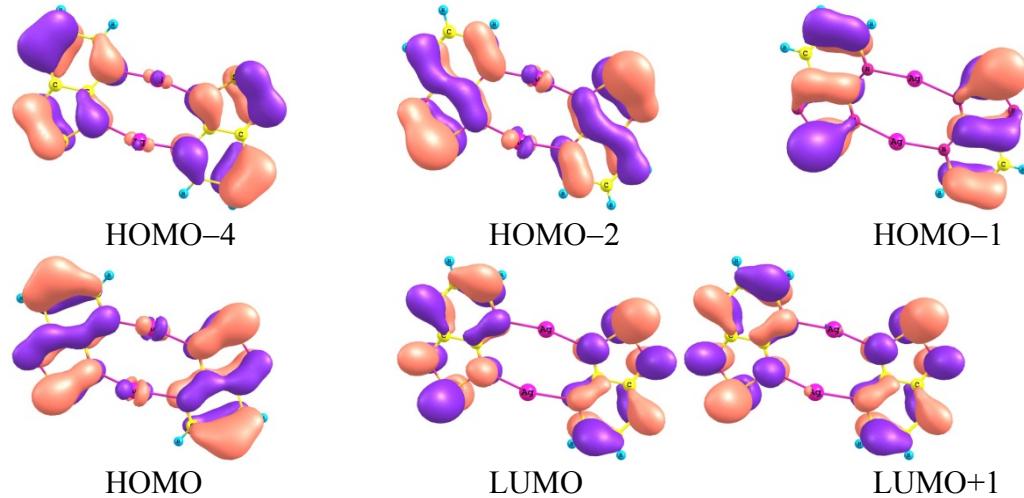


**Compound 9:**  $\lambda = 295$  nm ( $f = 0.312$ );

The major contributing MO's are shown below:

HOMO-4 → LUMO+1; HOMO-2 → LUMO; HOMO-1 → LUMO+1

HOMO → LUMO



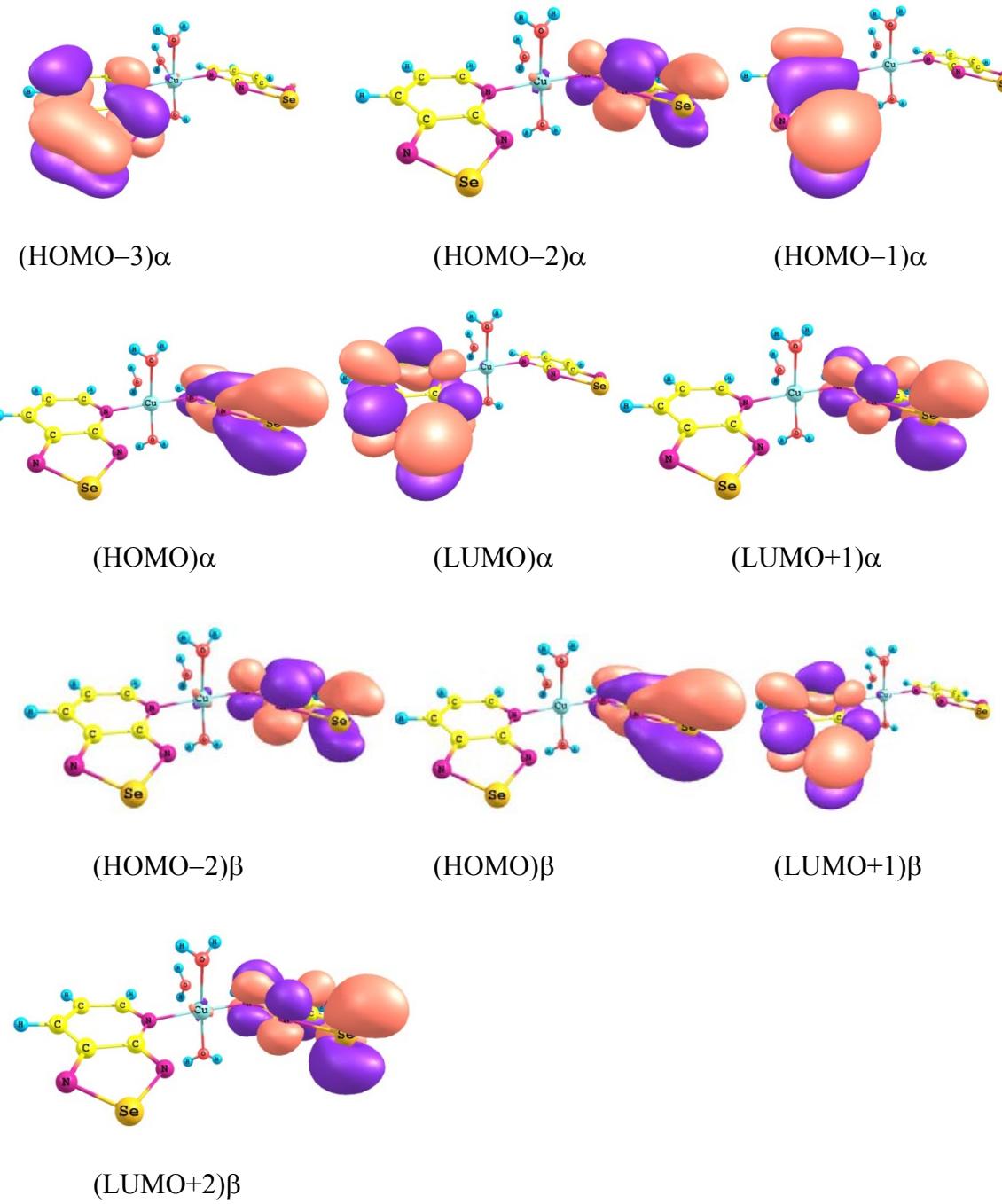
**Compound 13:**  $\lambda = 293$  nm ( $f = 0.321$ ); and  $786$  nm ( $f = 0.0001$ );

For transition at 293 nm, the contributing MO's are as follows

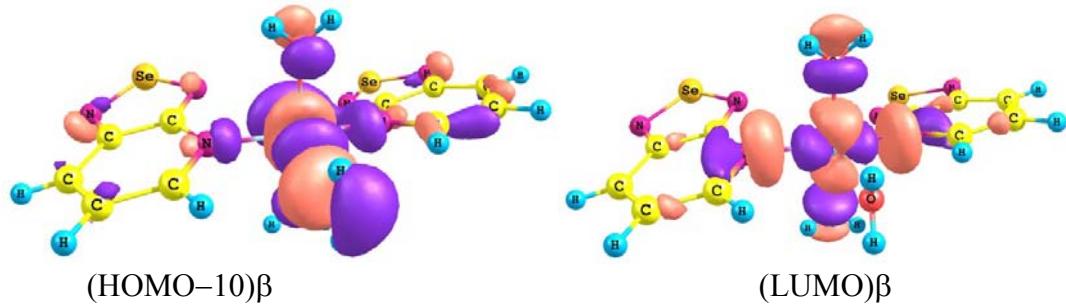
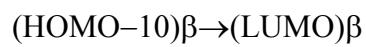
(HOMO-3) $\alpha$  $\rightarrow$ (LUMO) $\alpha$ ; (HOMO-2) $\alpha$  $\rightarrow$ (LUMO+1) $\alpha$ ; (HOMO-1) $\alpha$  $\rightarrow$ (LUMO) $\alpha$ ;

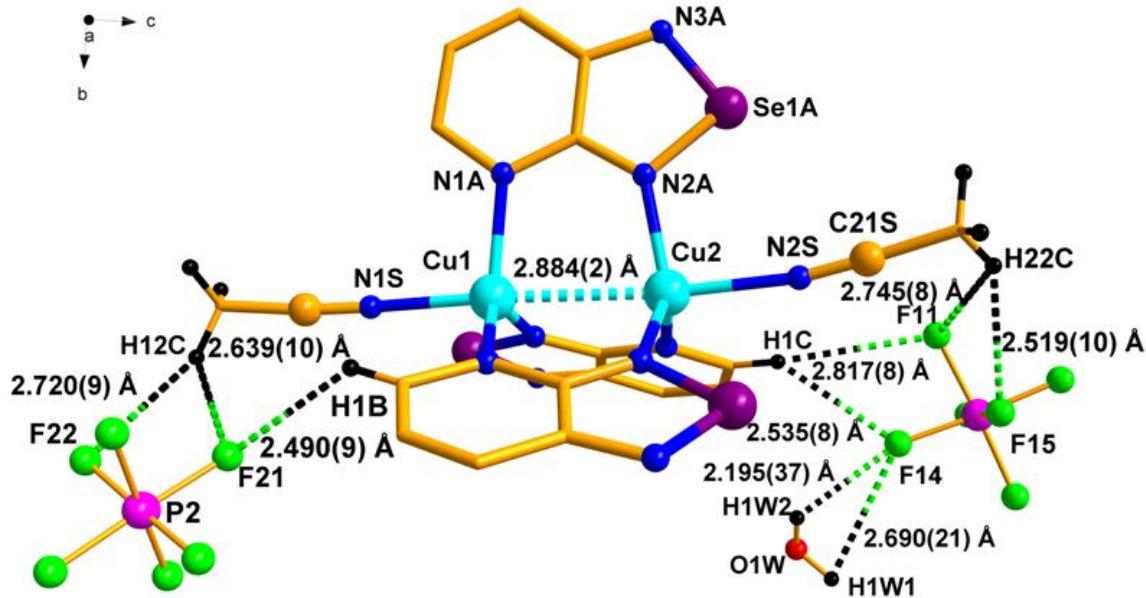
(HOMO) $\alpha$  $\rightarrow$ (LUMO+1) $\alpha$ ; (HOMO-2) $\beta$  $\rightarrow$ (LUMO+2) $\beta$ ; (HOMO-1) $\beta$  $\rightarrow$ (LUMO+1) $\beta$ ;

(HOMO) $\beta$  $\rightarrow$ (LUMO+2) $\beta$ ;

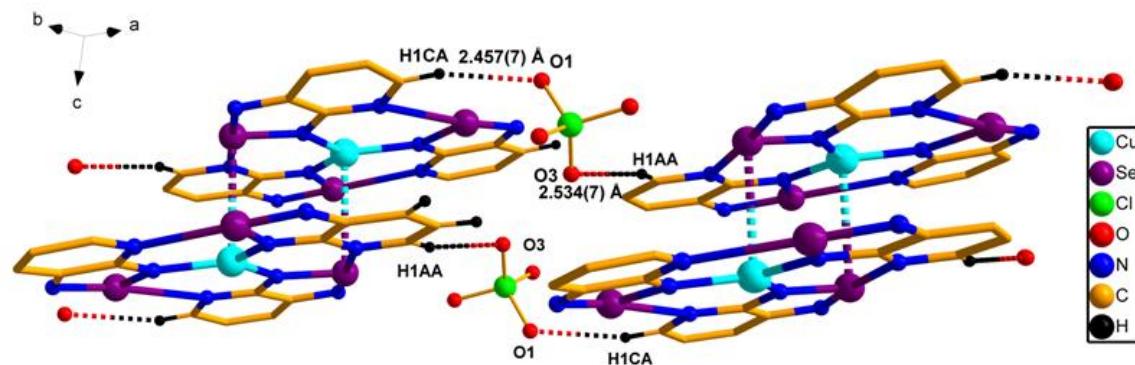


For transition at 786 nm, the contributing MO's are as follows





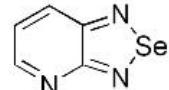
**Figure S15.** 1-D Supramolecular motif via C—H···F and H···F hydrogen bonding in the lattices of **6**. Only relevant hydrogen atoms are shown for clarity.



**Figure S16.** 1-D Supramolecular motif via C—H···O hydrogen bonding in the lattices of **8**. Only relevant hydrogen atoms are shown for clarity.

### Eager 300 Report

Page: 1 Sample: HBS-GM-PSD (HBS-GM-PSD)



Method Name : sp300307  
Method File : G:\eager300\Eager 300 EA1112\SP300307.mth  
Chromatogram : HBS-GM-PSD  
Operator ID : sp Company Name : C.E. Instruments  
Analysed : 03/26/2007 14:54 Printed : 3/26/2007 15:43  
Sample ID : HBS-GM-PSD (# 23) Instrument N. : Instrument #1  
Analysis Type : UnkNowN (Area) Sample weight : 1.835

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	23.0663	44	437473	RS	3.515000	.103357E+07
Carbon	32.5558	67	1537718	RS	1.000000	.256616E+07
Hydrogen	1.2850	181	140745	RS	10.925560	.596870E+07
Totals	56.9071		2115936			

Figure S17. Elemental analysis of 5.

### Eager 300 Report

Page: 1 Sample: GMCU-I (GMCU-I)

[Cu<sub>2</sub>(psd)<sub>3</sub>(CH<sub>3</sub>CN)<sub>2</sub>] 2PF<sub>6</sub>

Method Name : sp210807  
Method File : G:\eager300\Eager 300 EA1112\SP210807.mth  
Chromatogram : GMCU-I  
Operator ID : sp Company Name : C.E. Instruments  
Analysed : 08/21/2007 13:28 Printed : 8/21/2007 16:31  
Sample ID : GMCU-I (# 15) Instrument N. : Instrument #1  
Analysis Type : UnkNowN (Area) Sample weight : 1.703

Calib. method : using 'K Factors'

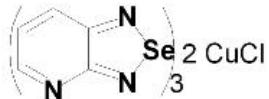
!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	14.2528	44	272496	FU	3.400539	.112265E+07
Carbon	21.8245	68	926632	FU	1.000000	.249315E+07
Hydrogen	0.8188	190	67237	RS	13.781580	.482178E+07
Totals	36.8961		1266365			

Figure S18. Elemental analysis of 6.

### Eager 300 Report

Page: 1 Sample: CG-A-19-10 (CG-A-19-10)



Method Name : SP040310  
 Method File : D:\CHNS2008\SP040310.mth  
 Chromatogram : CG-A-19-10  
 Operator ID : MP Company Name : C.E. Instruments  
 Analysed : 03/04/2010 13:03 Printed : 3/4/2010 14:57  
 Sample ID : CG-A-19-10 (# 17) Instrument N. : Instrument #1  
 Analysis Type : UnkNowN (Area) Sample weight : .968

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret. Time	Area	BC	Area ratio	K factor
Nitrogen	16.0849	43	201688	RS	3.143881	.129535E+07
Carbon	24.2663	67	634082	RS	1.000000	.267545E+07
Hydrogen	1.6114	172	155521	RS	4.077144	.695246E+07
Totals	41.9626		991290			

Figure S19. CH Analysis of Complexes 7.

### Eager 300 Report

Page: 1 Sample: CG-A-19-15 (CG-A-19-15)

[Cu<sub>2</sub>(psd)<sub>6</sub>] 2ClO<sub>4</sub>

Method Name : SP010410  
 Method File : D:\CHNS2008\SP010410.mth  
 Chromatogram : CG-A-19-15  
 Operator ID : MP Company Name : C.E. Instruments  
 Analysed : 04/01/2010 12:24 Printed : 4/1/2010 15:19  
 Sample ID : CG-A-19-15 (# 10) Instrument N. : Instrument #1  
 Analysis Type : UnkNowN (Area) Sample weight : .372

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret. Time	Area	BC	Area ratio	K factor
Nitrogen	17.8329	43	79667	RS	3.120633	.120092E+07
Carbon	25.6627	68	248612	RS	1.000000	.250885E+07
Hydrogen	1.1233	175	87932	RS	2.827315	.640465E+07
Totals	44.6190		416211			

Figure S20. CH Analysis of Complexes 8.

**Eager 300 Report**[Ag<sub>2</sub>(psd)<sub>2</sub>] 2NO<sub>3</sub>

Page: 1 Sample: HBSGM-Ag (HBSGM-Ag)

Method Name : sp130207R  
 Method File : G:\eager300\Eager 300 EA1112\SP130207R.mth  
 Chromatogram : HBSGM-Ag  
 Operator ID : MANOJA  
 Analysed : 02/13/2007 03:00  
 Sample ID : HBSGM-Ag (# 18)  
 Analysis Type : UnkNowN (Area)

Company Name : C.E. Instruments  
 Printed : 2/13/2007 10:19  
 Instrument N. : Instrument #1  
 Sample weight : 1.61

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret. Time	Area	BC	Area ratio	K factor
1	0.0000	7	77624	RS		0.0000
Nitrogen	15.7559	43	255175	RS	2.701908	.100593E+07
Carbon	17.0832	68	689458	RS	1.000000	.249398E+07
Hydrogen	0.5883	187	51368	RS	13.421940	.542356E+07
Totals	33.4274		1073625			

Figure S21. Elemental analysis of 9.

**Eager 300 Report**

Page: 1 Sample: HBS-GM-AgPSD (HBS-GM-AgPSD)

[Ag<sub>2</sub>(psd)<sub>2</sub>] 2CF<sub>3</sub>COOO

Method Name : sp300307  
 Method File : G:\eager300\Eager 300 EA1112\SP300307.mth  
 Chromatogram : HBS-GM-AgPSD  
 Operator ID : sp  
 Analysed : 03/26/2007 14:44  
 Sample ID : HBS-GM-AgPSD (# 22)  
 Analysis Type : UnkNowN (Area)

Company Name : C.E. Instruments  
 Printed : 3/26/2007 15:43  
 Instrument N. : Instrument #1  
 Sample weight : 2.474

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret. Time	Area	BC	Area ratio	K factor
Nitrogen	10.4302	44	266706	RS	4.943953	.103357E+07
Carbon	20.6954	67	1318580	RS	1.000000	.256616E+07
Hydrogen	0.5716	187	84413	RS	15.620570	.596870E+07
Totals	31.6973		1669698			

Figure S22. Elemental analysis of 10.

**Eager 300 Report**

Page: 1    Sample: CGA19-4 (CGA19-4)                   $[\text{Cu}(\text{psd})_4(\text{H}_2\text{O})_3] \text{2ClO}_4$

Method Name : SP290110  
 Method File : D:\CHNS2008\SP290110.mth  
 Chromatogram : CGA19-4  
 Operator ID : SP    Company Name : C.E. Instruments  
 Analysed : 01/29/2010 15:10                              Printed : 1/29/2010 16:35  
 Sample ID : CGA19-4 (# 30)                              Instrument N. : Instrument #1  
 Analysis Type : UnkNowN (Area)                         Sample weight : .469

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret. Time	Area	BC	Area ratio	K factor
Nitrogen	15.8810	43	83258	RS	3.372543	.111783E+07
Carbon	22.5965	68	280790	RS	1.000000	.264952E+07
Hydrogen	1.1410	187	42659	RS	6.582187	.592042E+07
Totals	39.6185		406706			

Figure S23. CH Analysis of Complexes 11.

**Eager 300 Report**

Page: 1    Sample: CGA19-5-2 (CGA19-5-2)                   $[\text{Cu}(\text{psd})_4(\text{H}_2\text{O})] \text{2ClO}_4(\text{CHCl}_3)$

Method Name : SP290110  
 Method File : D:\CHNS2008\SP290110.mth  
 Chromatogram : CGA19-5-2  
 Operator ID : SP    Company Name : C.E. Instruments  
 Analysed : 01/29/2010 13:12                              Printed : 1/29/2010 16:32  
 Sample ID : CGA19-5-2 (# 19)                              Instrument N. : Instrument #1  
 Analysis Type : UnkNowN (Area)                         Sample weight : .763

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret. Time	Area	BC	Area ratio	K factor
1	0.0000	18	5442	RS		0.0000
Nitrogen	14.6562	43	125003	RS	3.601458	.111783E+07
Carbon	22.2693	68	450193	RS	1.000000	.264952E+07
Hydrogen	1.0546	184	58618	RS	7.680115	.592042E+07
Totals	37.9802		639256			

Figure S24. CH Analysis of Complexes 12.

**Eager 300 Report**[Cu(psd)4(H<sub>2</sub>O)<sub>4</sub>] 2NO<sub>3</sub>

Page: 1 Sample: HBS-GM-CUNO3 (HBS-GM-CUNO3)

Method Name : sp200307  
Method File : G:\eager300\Eager 300 EA1112\SP200307.mth  
Chromatogram : HBS-GM-CUNO3  
Operator ID : MANOJA Company Name : C.E. Instruments  
Analysed : 03/11/2007 10:43 Printed : 3/11/2007 16:57  
Sample ID : HBS-GM-CUNO3 (# 26) Instrument N. : Instrument #1  
Analysis Type : UnkNowN (Area) Sample weight : 2.332

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret. Time	Area	BC	Area ratio	K factor
Nitrogen	20.4559	45	485811	RS	2.992232	.101841E+07
Carbon	24.2050	68	1453659	RS	1.000000	.254181E+07
Hydrogen	1.4374	178	198990	RS	7.305186	.593640E+07
Totals	46.0983		2138460			

**Figure S25.** Elemental analysis of 13.**Eager 300 Report**Page: 1 Sample: RCS-303 (RCS-303) [Co(psd)4(H<sub>2</sub>O)<sub>4</sub>] (ClO<sub>4</sub>)<sub>2</sub>

Method Name : SD080911  
Method File : D:\CHNS2011\SD080911.mth  
Chromatogram : RCS-303  
Operator ID : SD Company Name : C.E. Instruments  
Analysed : 09/08/2011 14:18 Printed : 9/8/2011 16:03  
Sample ID : RCS-303 (# 21) Instrument N. : Instrument #1  
Analysis Type : UnkNowN (Area) Sample weight : 1.066

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

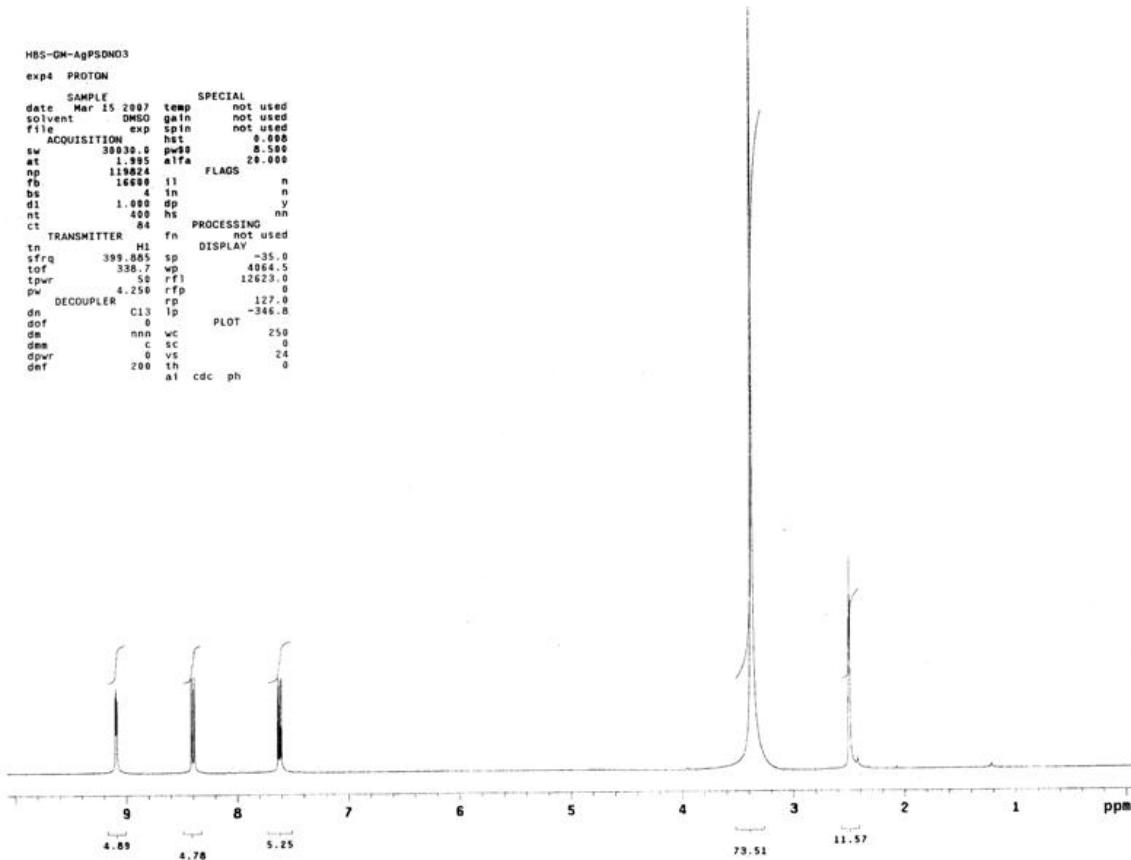
Element Name	%	Ret. Time	Area	BC	Area ratio	K factor
Nitrogen	12.9064	43	210796	FU	2.880464	.153215E+07
Carbon	22.9596	67	607189	FU	1.000000	.248087E+07
Hydrogen	1.8123	181	117413	RS	5.171398	.607763E+07
Totals	37.6782		935398			

**Figure S26.** Elemental analysis of 14.

```

HBS-GM-AgPSDNO3
exp4 PROTON
      SAMPLE          SPECIAL
date Mar 15 2007 temp not used
solvent   DMSO gain not used
file      exp1 tbin not used
ACQUISITION hst    8.000
sw       30030.0 pw90  8.500
at        1.995 alfa  20.000
rt       11982.0 flags
fb       16500 il   n
bs        4 in   n
di       1.000 dp   y
nt       400 hs   nn
ct        84 PROCESSING
TRANSMITTER HI   not used
tn        H1   DISPLAY
tfrq    399.864 sp   -35.0
tot      33.7 sp   4054.5
tpwr    5e rfp  12623.0
pw     4.250 rfp  0
DECOUPLER C13 1p   127.0
dn        0 PLOT -346.8
dof      nnn wc   250
dm       c sc   0
dpwr    0 ts   24
dprf    200 th   0
dgrf    ai cdc ph

```



**Figure S27.**  $^1\text{H}$  NMR spectrum of **9** in  $\text{DMSO-d}_6$ .

HBS-GH-AgPSDTFA [Ag(psdi)<sub>2</sub>](CF<sub>3</sub>COO)<sub>2</sub>

exp4 PROTON

```

SAMPLE          SPECIAL
date  Mar 27 2007 temp    not used
solvent   DMSO gain    not used
file     /export/home/~ spin   not used
ACQUISITION   pw1    8.395
              pw2b   8.595
sw      30039.8 pdd   20.000
at      1.000 alfa   20.000
np      115000   flags
fb      100000   11    n
bs      10000   4    in    n
d1      1.000 dp    y
nt      400 hs    n
ct      92   PROCESSING
TRANSMITTER   H1   not used
tn      H1   DISPLAY
sfrq   399.885 sp   -114.2
t0f    338.885 wp   4225.1
tpwr   50 r1    13625.1
pw    4.250 rfp   399.7
p0    1.000   flags
DECOUPLER    C13 lp   -392.8
dn      C13 lp   -392.8
dof    0   PLOT
ds      minn wc   250
dm      c sc    0
dpwr   0 vs    17
dmf    200 th    5
ai      cdc ph

```

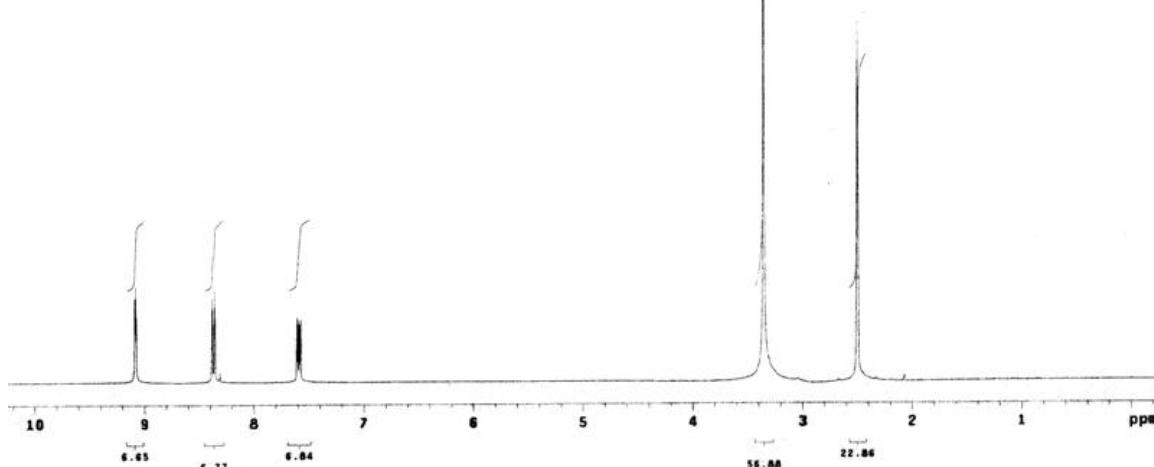


Figure S28. <sup>1</sup>H NMR spectrum of **10** in DMSO-d<sub>6</sub>.

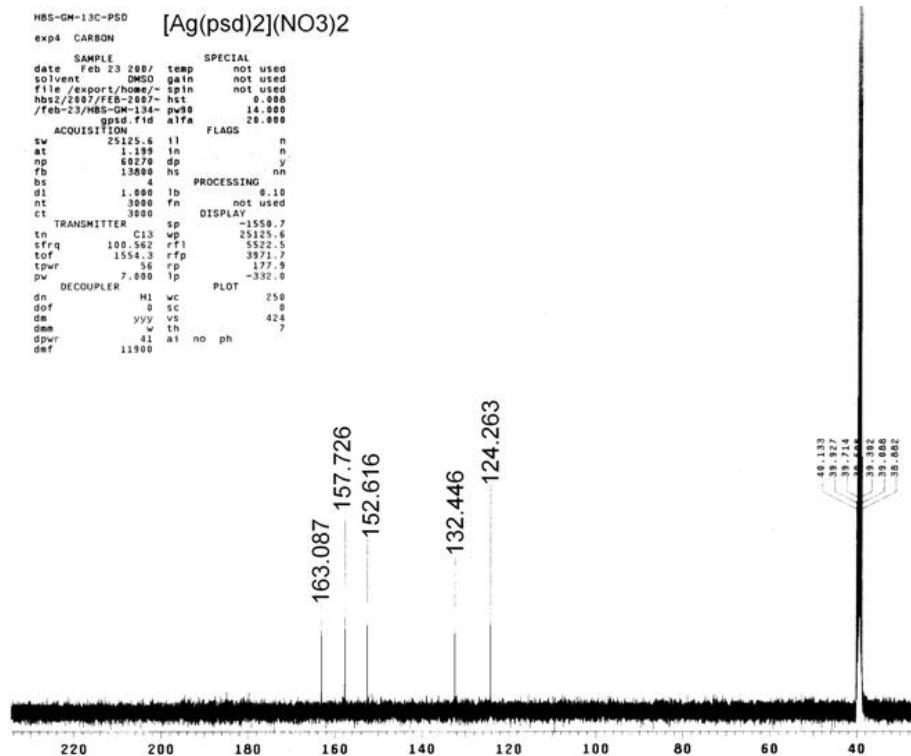
HBS-GM-13C-PSD [Ag(psdi)<sub>2</sub>](NO<sub>3</sub>)<sub>2</sub>

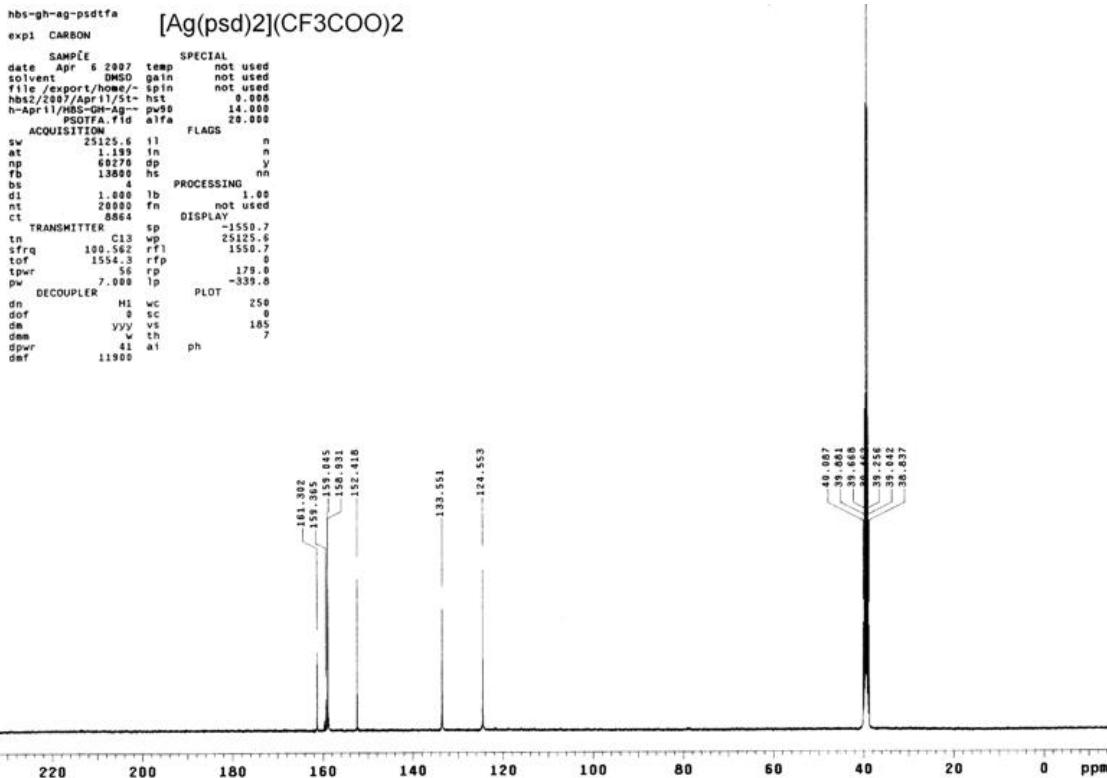
exp4 CARBON

```

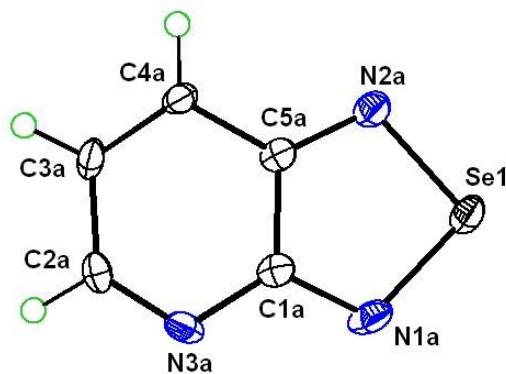
SAMPLE          SPECIAL
date  Feb 23 2007 temp    not used
solvent   DMSO gain    not used
file     /export/home/~ spin   not used
hbs2/2807/FEB-2007- hst   0.000
/feb-23/HBS-GM-13C- psd   14.000
psd.fid  psd   20.000
         gpsd.fid alfa   20.000
ACQUISITION   pw1    1550.7
              pw2b   1550.7
              flags
sw      25125.0 1b    8.10
at      1.000   1h    n
np      60270   dp    nn
fb      136000   hs    nn
br      1.000   1b    8.10
di      1.000   1b    8.10
nt      30000   fm    not used
ct      3000   DISPLAY
TRANSMITTER   H1   not used
tn      C13 lp   25125.6
tfrq   100.562 r1f   5522.5
t0f    1554.3 rfp   3971.7
tpwr   50 rfp   177.9
pw    7.000 lp   -392.0
p0    1.000   flags
DECOUPLER    C13 lp   -392.0
dn      C13 lp   -392.0
dof    0   PLOT
ds      vvv vs    424
dm      w th    7
dpwr   41 ai    no ph
dmf    11900

```

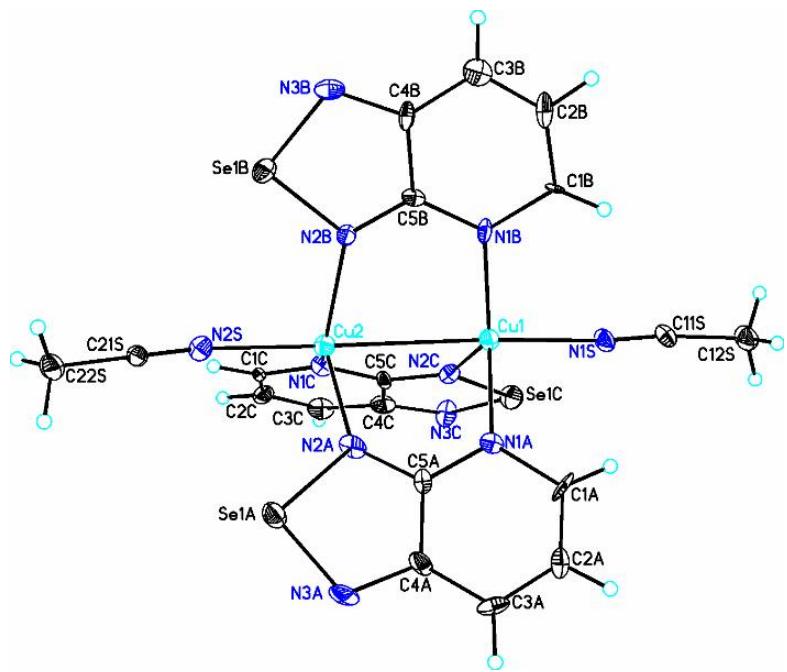




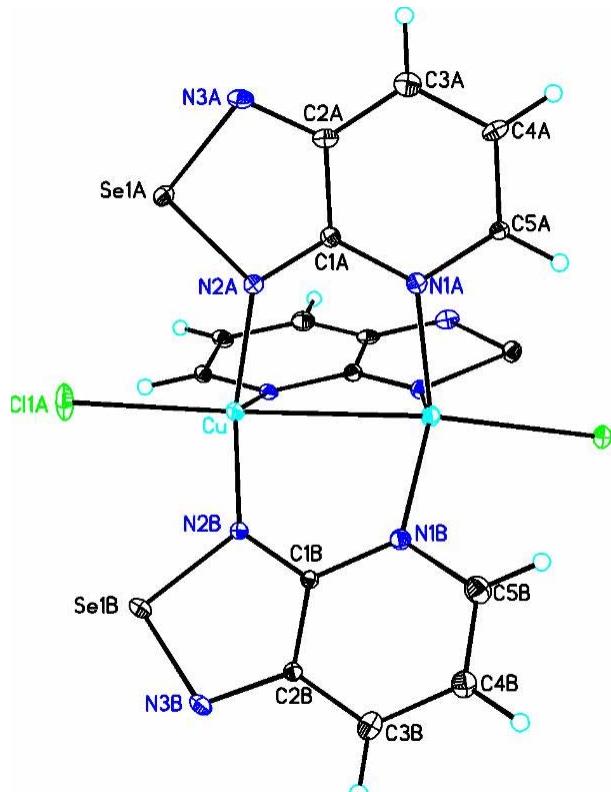
**Figure S30.**  $^{13}\text{C}$  NMR spectrum of **10** in  $\text{DMSO-d}_6$ .



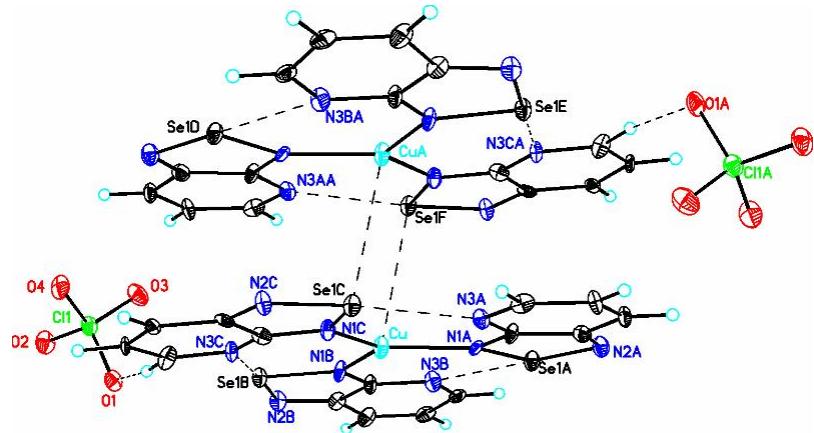
**Figure S31.** ORTEP diagram of **5**.



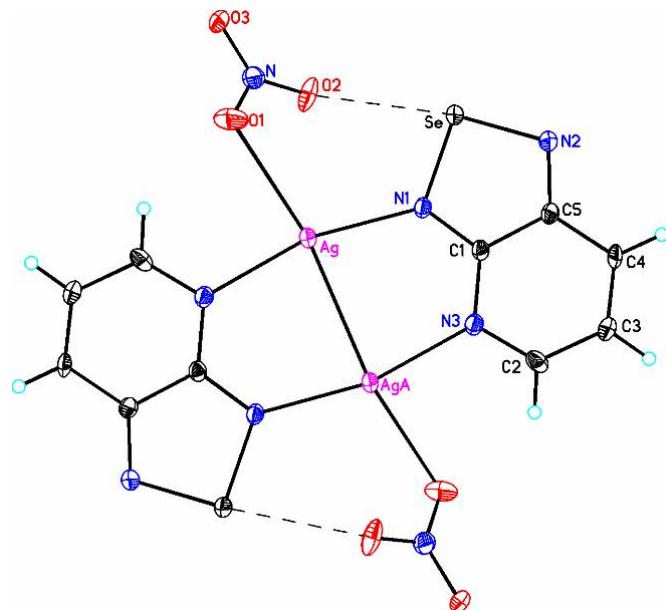
**Figure S32.** ORTEP diagram of the cationic part of **6**.



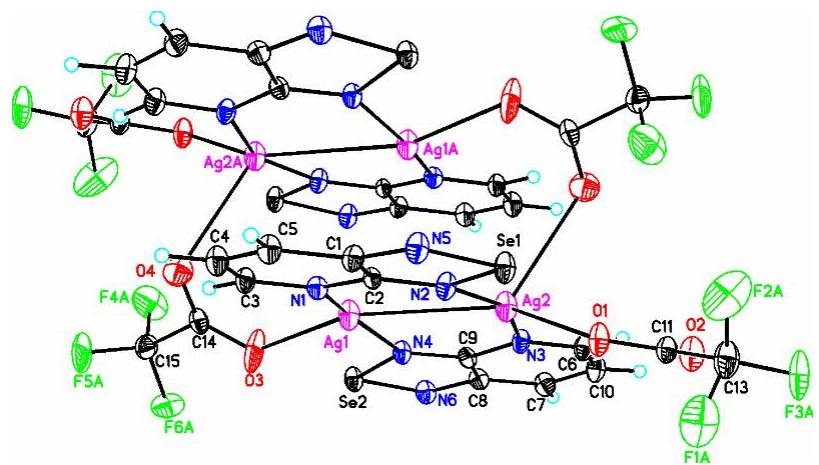
**Figure S33.** ORTEP diagram of the **7**.



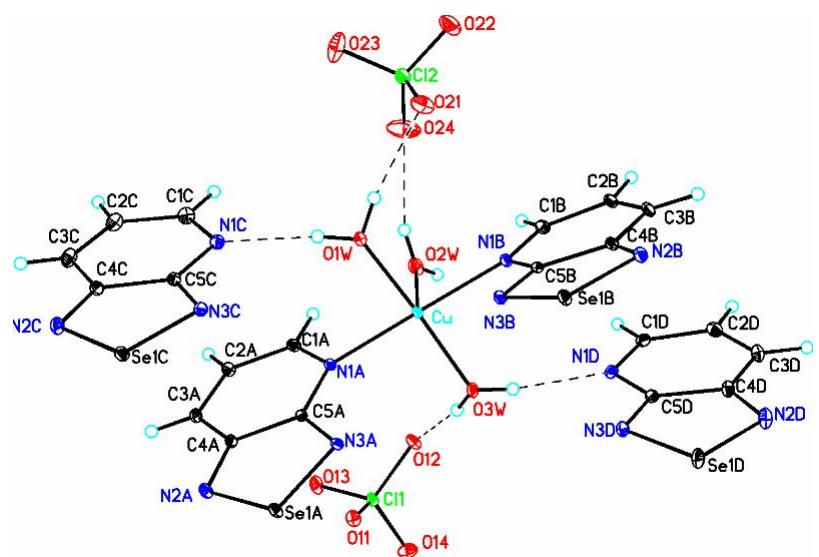
**Figure S34.** ORTEP diagram of **8**.



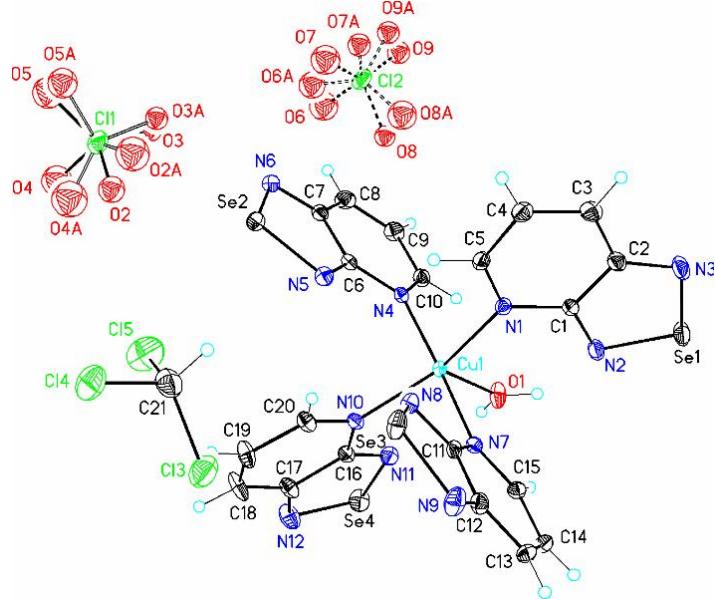
**Figure S35.** ORTEP diagram of **9**.



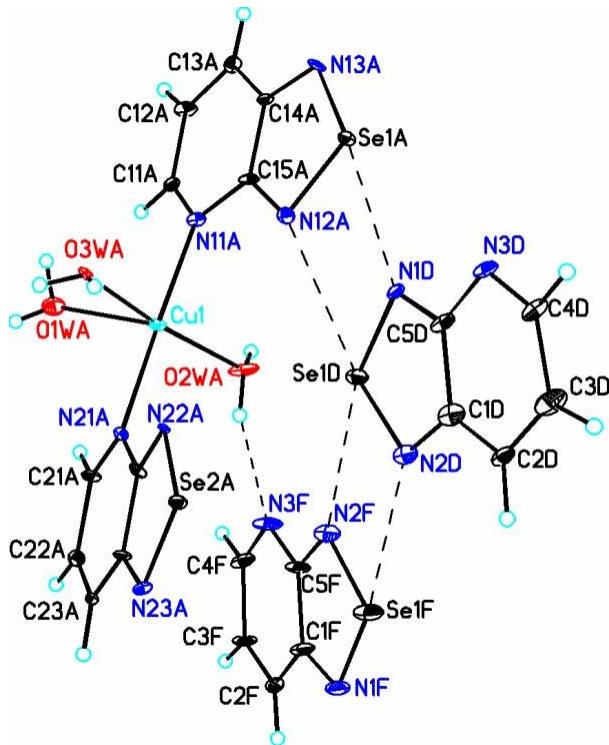
**Figure S36.** ORTEP diagram of 10.



**Figure S37.** ORTEP diagram of 11.

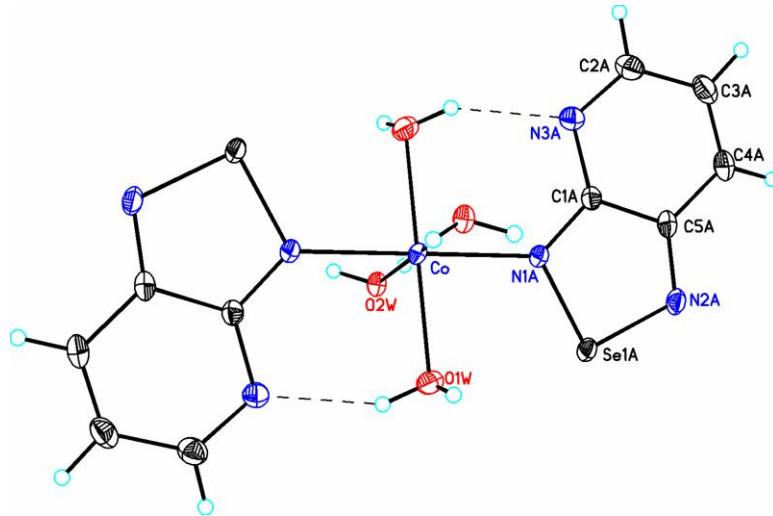


**Figure S38.** ORTEP diagram of **12**.



**Figure S39.** ORTEP diagram of the cationic part of **13**. Selected bond distances [Å] and angles [°]: Cu(2)–N(11B) 2.038(5), Cu(2)–N(21B) 2.060(5), Cu(2)–O(1WB) 2.259(4), Cu(2)–O(2WB) 1.956(3), Cu(2)–O(3WB) 1.927(3), Se(2B)•••N(1C) 2.877(5), Se(1C)•••N(2B) 3.031(5), Se(1C)•••N(1E) 3.031(5).

3.006(6), Se(1E)…N(2C) 2.869(6), O(2WB)–H(2WD)…N(2E) 2.035(5);,  
 O(1WB)–Cu(2)–O(3WB) 100.59(17), O(1WB)–Cu(2)–O(2WB)  
 96.67(19), O(2WB)–Cu(2)–O(3WB) 162.7(2).



**Figure S40.** ORTEP diagram of the cationic part of **14**.

Table S3. Hydrogen bonds for **6**, **8** to **14** [Å and °].

D–H…A	d(D–H)	d(H…A)	d(D…A)	∠(DHA)	Symmetry
<b>6</b>					
O(1W)–H(1W1)…F(33)	0.822(18)	2.40(2)	3.187(18)	159(4)	x+1/2,-y+3/2,-z+1
O(1W)–H(1W1)…F(32)	0.822(18)	2.65(3)	3.242(18)	131(3)	x+1/2,-y+3/2,-z+1
O(1W)–H(1W2)…F(14)	0.823(17)	2.20(4)	2.663(17)	116(4)	
O(1W)–H(1W2)…Se(1E)	0.823(17)	2.54(4)	2.913(15)	109(4)	-x+3/2,y+1/2,z
<b>8</b>					
C(1A)–H(1AA)…O(3)	0.95	2.53	3.451(12)	162.4	x+1/2,y+1/2,z
C(2A)–H(2AA)…O(3)	0.95	2.62	3.504(12)	155.4	-x+1,-y+1,-z+1
C(3B)–H(3BA)…O(1)	0.95	2.53	3.405(13)	153.1	-x+1/2,y-1/2,-z+3/2
C(1C)–H(1CA)…O(1)	0.95	2.46	3.384(12)	164.7	
C(3C)–H(3CA)…O(1)	0.95	2.52	3.149(12)	123.8	-x+1/2,y+1/2,-z+3/2
<b>9</b>					
C(2)–H(2A)…O(1)	0.95	2.42	3.138(4)	132.2	-x+1,-y+1,-z+1
C(3)–H(3A)…O(3)	0.95	2.45	3.146(4)	129.8	x+1/2,-y+1/2,z+1

C(3)–H(3A)…N(2)	0.95	2.55	3.449(4)	158.3	-x+3/2,y+1/2,-z+2
<b>10</b>					
C(3)–H(3A)…O(4)	0.95	2.46	3.297(7)	147.2	
C(4)–H(4A)…O(2)	0.95	2.49	3.412(7)	164.0	x,y,z+1
C(5)–H(5A)…F(3A)	0.95	2.54	3.134(7)	120.4	x,y,z+1
C(5)–H(5A)…F(6B)	0.95	2.28	3.193(7)	161.5	x-1,y-1,z
C(7)–H(7A)…F(2A)	0.95	2.39	3.290(8)	158.4	x+1,y+1,z
<b>11</b>					
O(1W)–H(1W1)…N(1C)	0.808(17)	1.908(17)	2.710(3)	172(3)	-x+1,-y+1,-z+1
O(1W)–H(1W2)…O(21)	0.819(16)	2.023(18)	2.822(3)	165(3)	
O(2W)–H(2W1)…O(22)	0.826(17)	2.149(18)	2.966(4)	170(3)	-x,-y+1,-z
O(2W)–H(2W2)…O(24)	0.784(17)	2.06(2)	2.807(3)	158(4)	
O(3W)–H(3W1)…N(1D)	0.798(17)	1.959(17)	2.746(3)	169(3)	
O(3W)–H(3W2)…O(12)	0.828(16)	1.961(17)	2.781(3)	171(3)	
<b>12</b>					
O(1)–H(1OB)…N(2)	0.84(2)	2.28(4)	2.778(6)	118(4)	
O(1)–H(1OB)…O(8)	0.84(2)	2.33(3)	3.133(8)	158(5)	-x+1,-y,-z
O(1)–H(1OA)…O(2)	0.84(2)	2.44(4)	3.209(9)	153(5)	x,y-1,z
O(1)–H(1OA)…N(11)	0.84(2)	2.22(4)	2.798(6)	126(4)	
C(5)–H(5)…N(5)	0.95	2.59	3.378(6)	141.0	
C(8)–H(8)…O(8)	0.95	2.58	3.149(9)	118.9	
C(9)–H(9)…O(8)	0.95	2.49	3.118(9)	123.5	
C(10)–H(10)…O(1)	0.95	2.43	3.051(7)	123.1	
C(13)–H(13)…O(6)	0.95	2.49	3.363(11)	152.7	x+1,y,z
C(15)–H(15)…O(1)	0.95	2.51	3.107(7)	121.1	
C(15)–H(15)…O(9)	0.95	2.57	3.294(10)	133.3	-x+1,-y,-z
C(20)–H(20)…N(8)	0.95	2.51	3.188(6)	128.5	
C(21)–H(21)…O(9)	1.00	2.26	3.177(10)	152.5	-x+1,-y+1,-z
<b>13</b>					
O(1WA)–H(1WB)…O(23S)	0.82	2.09	2.896(10)	166.1	
O(1WC)–H(1WE)…O(23T)	0.82	2.06	2.794(12)	148.7	-x+1,-y+2,-z+1
O(2WA)–H(2WB)…O(1W)	0.82	1.88	2.674(8)	163.1	
O(3WA)–H(3WA)…N(22A)	0.82	2.67	3.185(6)	122.5	
O(3WA)–H(3WB)…O(21T)	0.82	1.90	2.597(11)	142.4	
O(3WA)–H(3WB)…O(21S)	0.82	2.09	2.807(8)	146.1	

O(3WA)–H(3WB)···O(23T)	0.82	2.41	3.169(11)	155.2	
O(1WB)–H(1WC)···O(33S)	0.82	2.07	2.821(11)	152.2	
O(1WB)–H(1WC)···O(32T)	0.82	2.28	2.924(16)	136.2	
O(1WB)–H(1WC)···O(32S)	0.82	2.53	3.103(12)	128.4	
O(1WB)–H(1WC)···O(33T)	0.82	2.45	3.261(17)	168.2	
O(1WB)–H(1WD)···O(12S)	0.82	2.01	2.812(7)	167.2	
O(2WB)–H(2WC)···O(43S)	0.82	1.97	2.790(8)	176.1	
O(3WB)–H(3WC)···O(11S)	0.82	2.04	2.718(7)	140.0	-x,-y+1,-z+2
O(1W)–H(1W1)···O(42S)	0.82	1.94	2.639(12)	142.0	x+1,y,z
O(1W)–H(1W2)···O(31S)	0.82	2.42	3.065(12)	136.5	x+1,y,z
O(1W)–H(1W2)···O(33T)	0.82	2.36	2.877(18)	121.8	x+1,y,z
O(1W)–H(1W2)···O(31T)	0.82	1.90	2.605(14)	142.9	x+1,y,z
O(2W)–H(2W1)···O(22S)	0.82	2.10	2.825(19)	148.1	-x,-y+2,-z+1
O(2W)–H(2W2)···O(43S)	0.82	1.97	2.583(15)	131.4	
<b>14</b>					
O(1W)–H(1W1)···N(3A)	0.826(18)	2.02(3)	2.767(4)	151(3)	-x+1,-y+2,-z+1
O(1W)–H(1W2)···N(1C)	0.805(18)	2.55(3)	3.267(5)	150(4)	-x+1,-y+2,-z+1
O(1W)–H(1W2)···O(1A)	0.805(18)	2.60(2)	3.145(8)	126(2)	x-1,y+1,z
O(2W)–H(2W1)···N(3C)	0.799(17)	2.006(17)	2.799(4)	172(4)	
O(2W)–H(2W2)···N(3B)	0.817(17)	1.974(18)	2.790(4)	176(3)	
C(4A)–H(4AA)···O(4A)	0.93	2.62	3.118(7)	114.1	
C(2B)–H(2BA)···O(1A)	0.93	2.56	3.367(7)	145.1	-x+2,-y+1,-z+1
C(4B)–H(4BA)···O(4B)	0.93	2.23	3.148(7)	169.7	
C(4C)–H(4CA)···O(3A)	0.93	2.58	3.278(6)	132.4	x-1,y+1,z-1
C(2C)–H(2CA)···O(2W)	0.93	2.53	3.380(5)	152.6	-x,-y+2,-z+1