Supporting Information for

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

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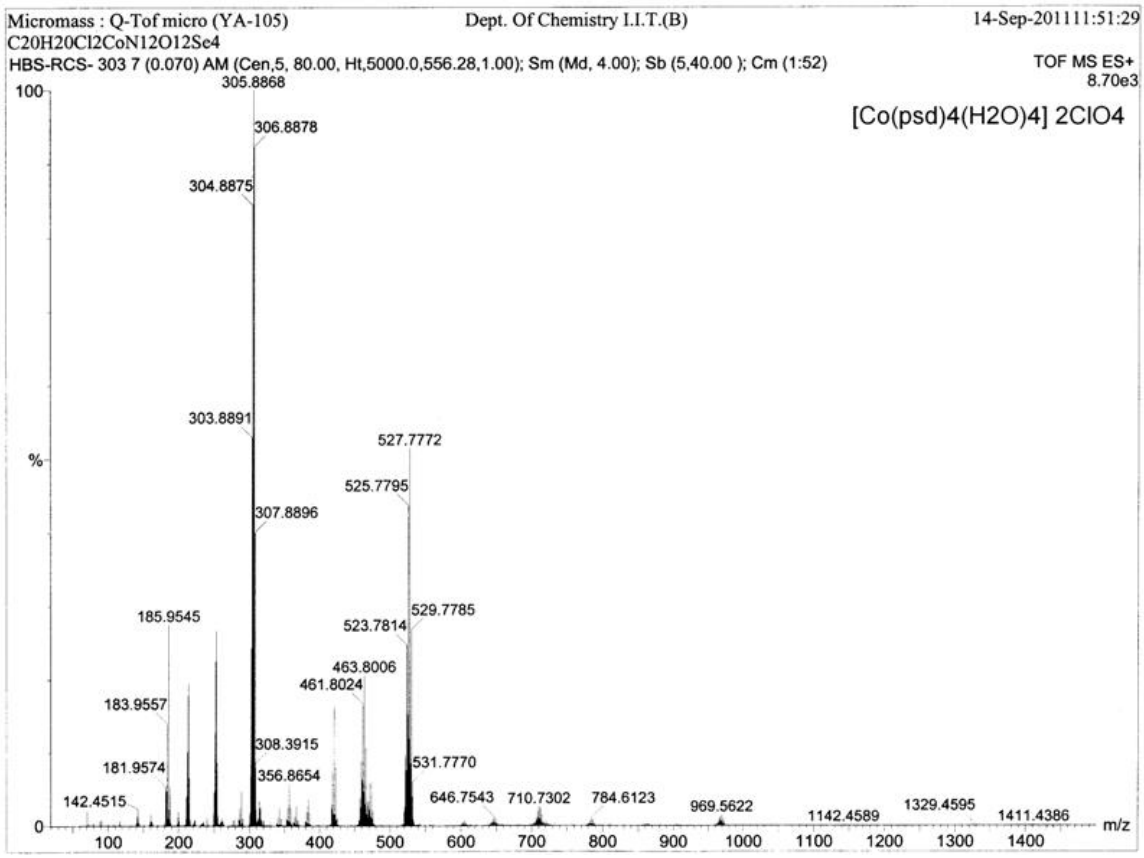

Figure S1. ESI spectrum of **14.**

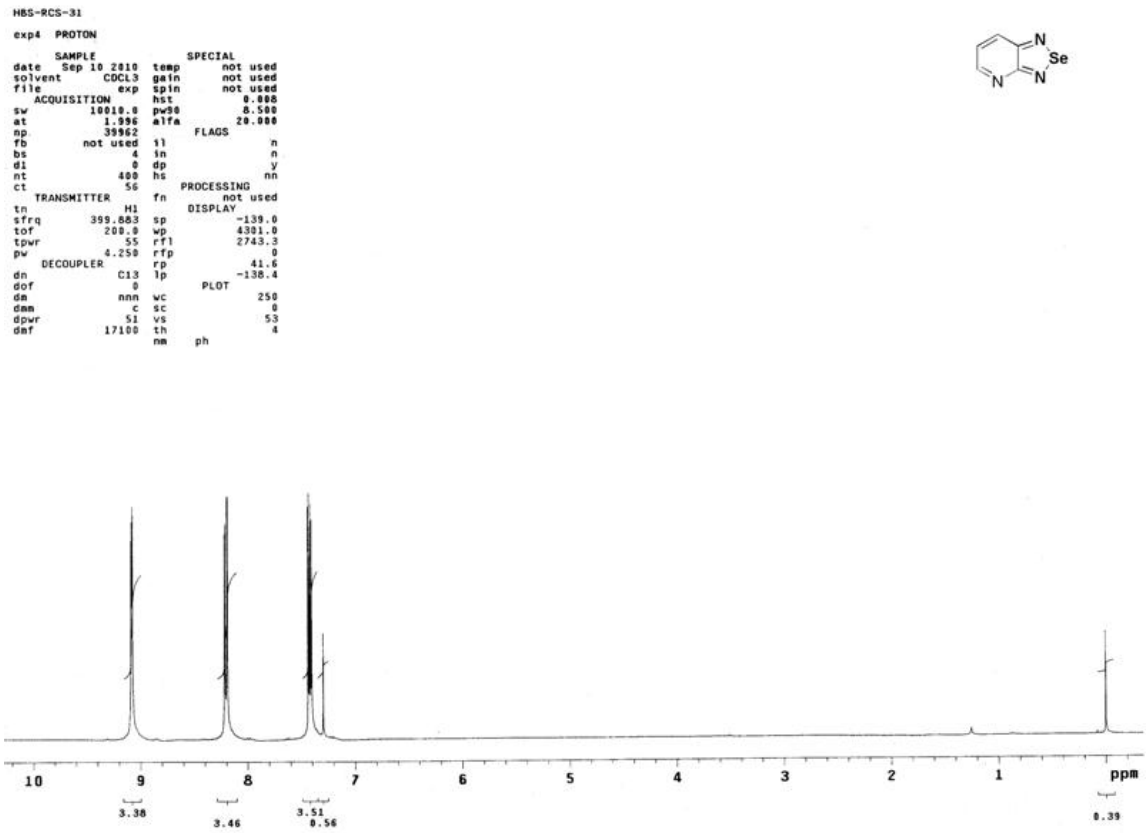

Figure S2. ^{1}H NMR spectrum of **5** in $CDCl_3$.

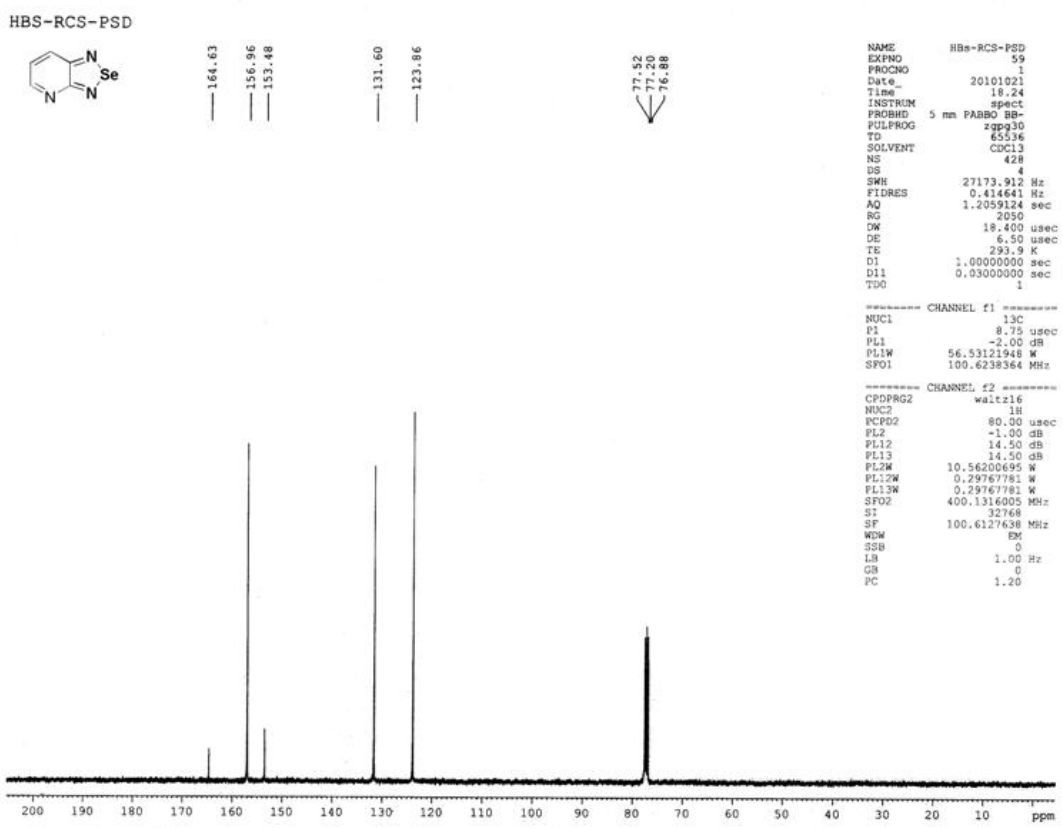

Figure S3. ^{13}C NMR spectrum of **5** in $CDCl_3$.

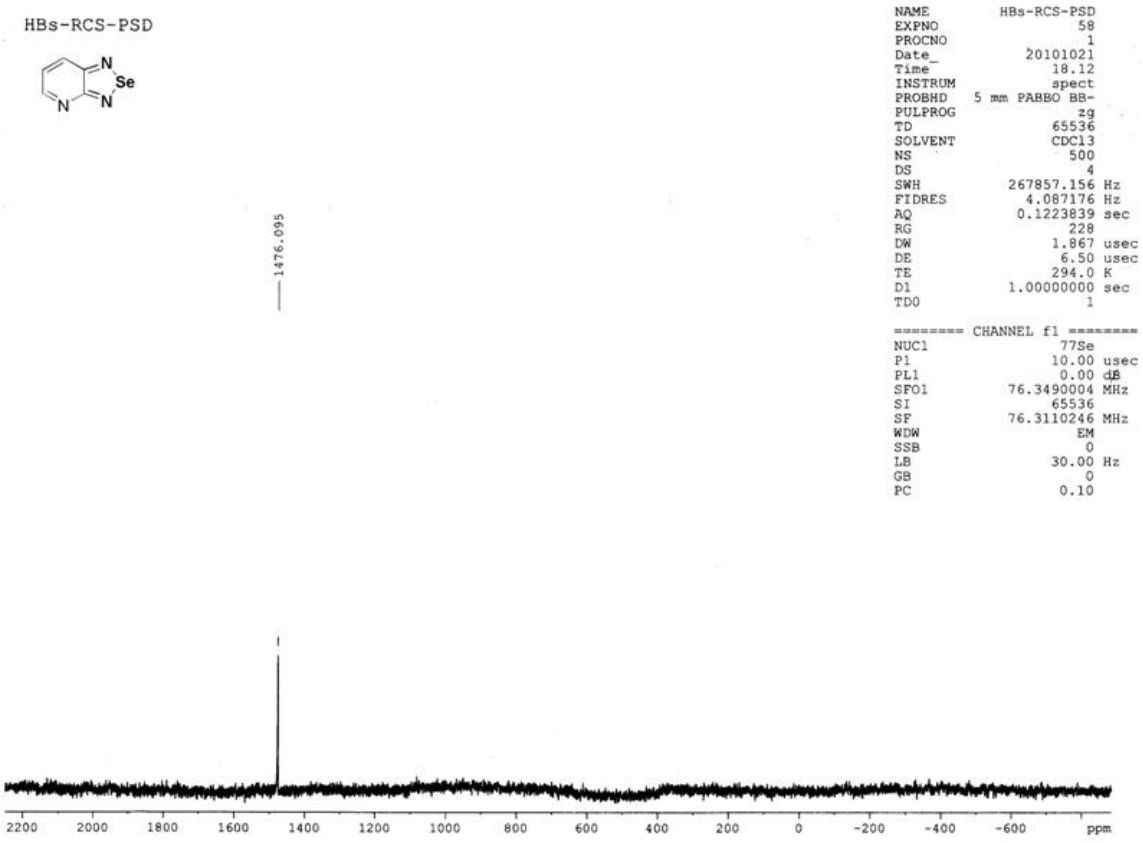

Figure S4. ^{77}Se NMR spectrum of **5** in $CDCl_3$.

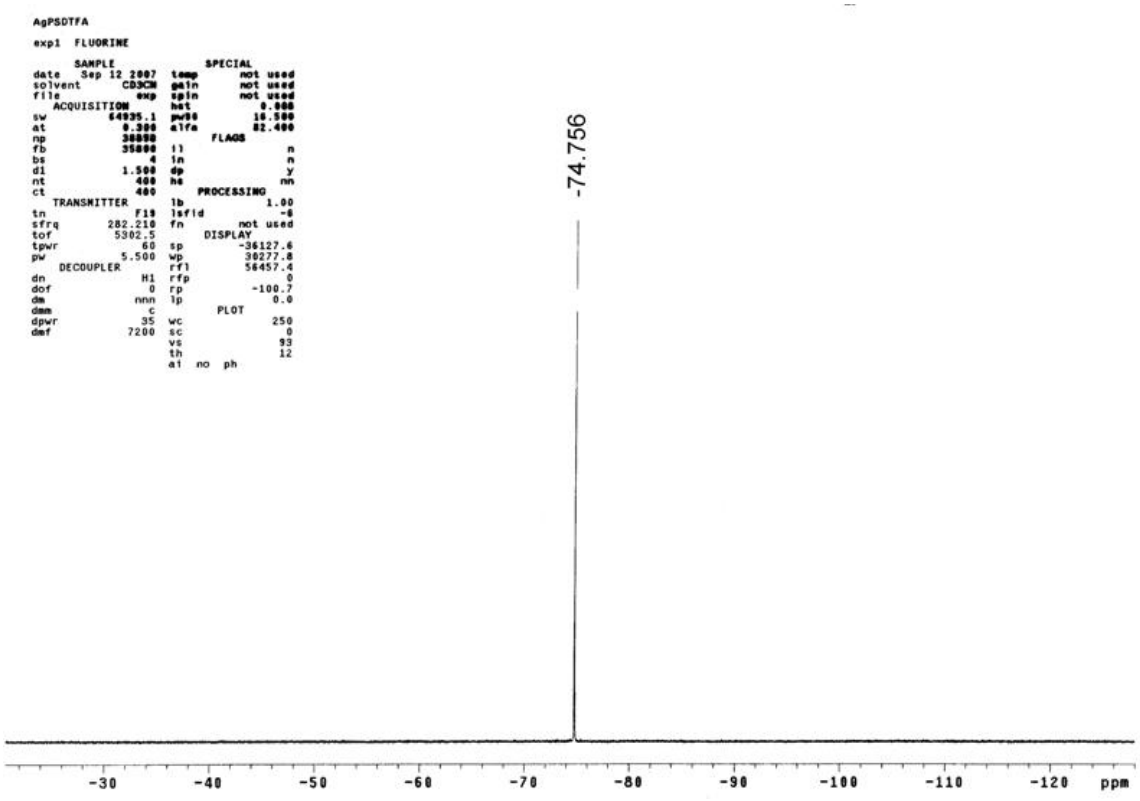

Figure S5. ^{19}F NMR Spectrum of **10** in CD_3CN.

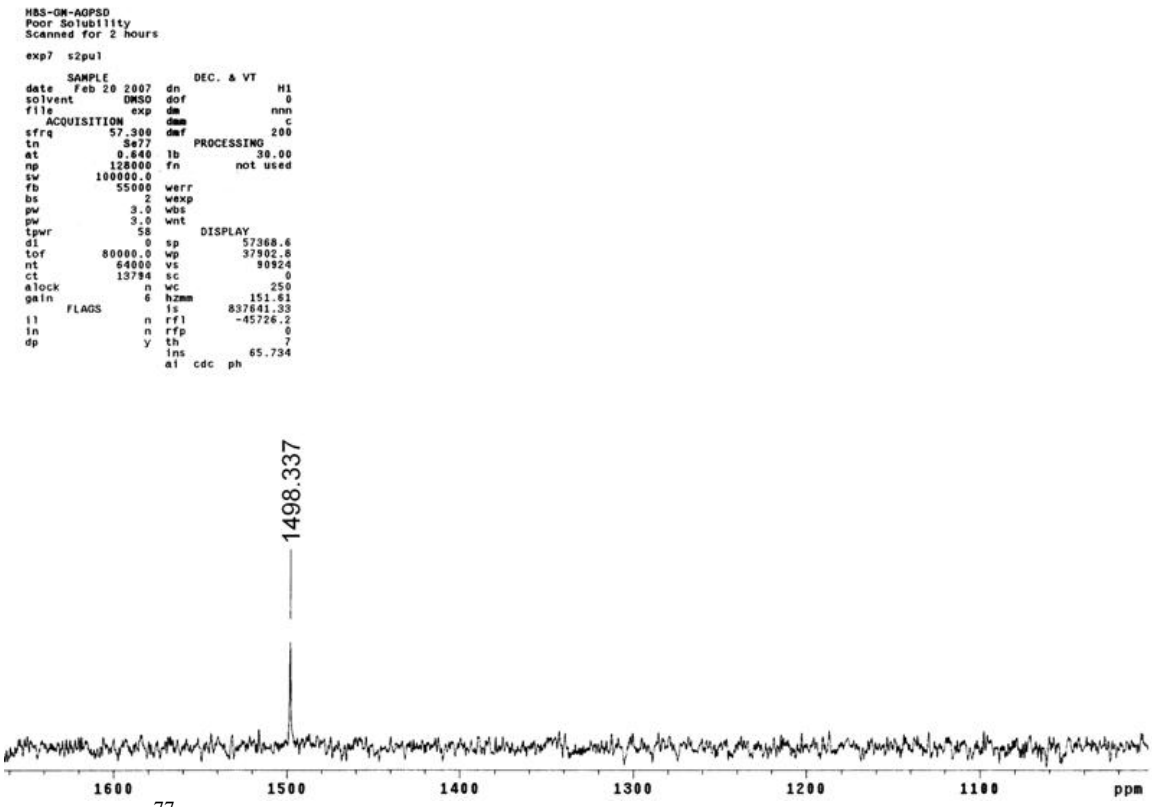

Figure S6. ^{77}Se NMR spectrum of **9** in DMSO-d_6.

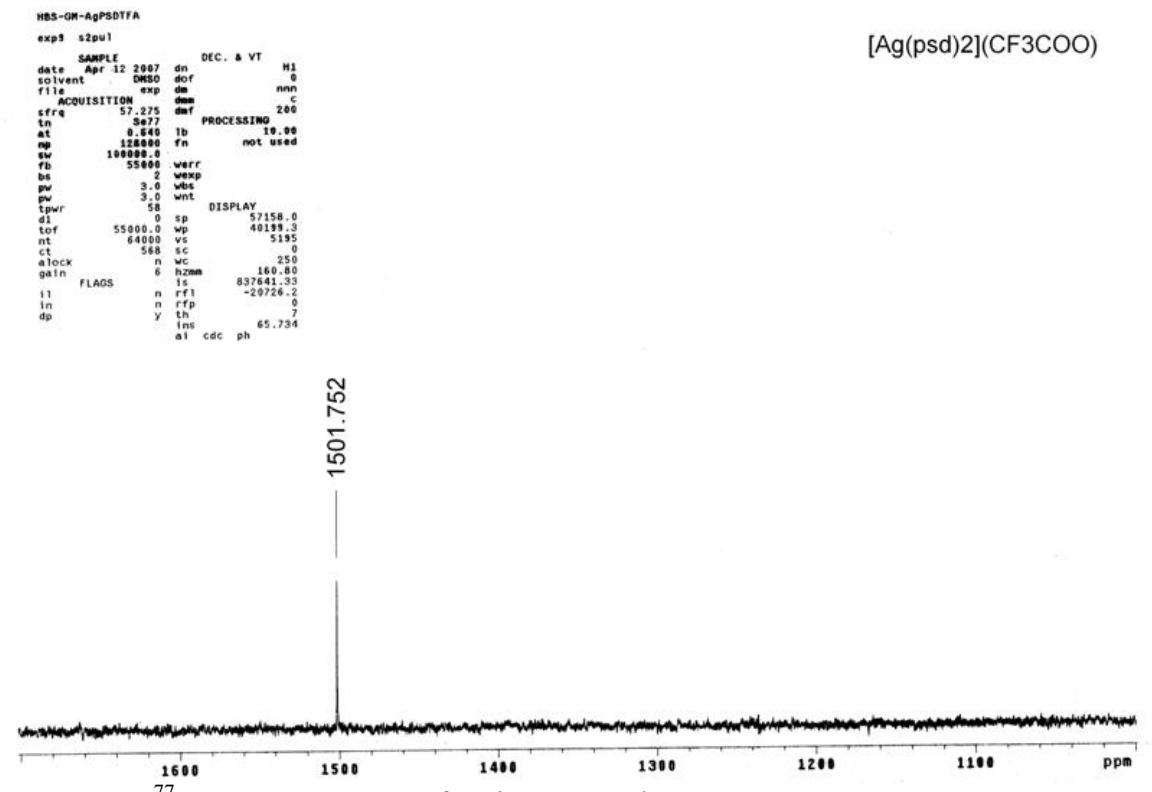

Figure S7. ^{77}Se NMR spectrum of **10** in DMSO-d_6.

Table S1. UV spectrum of Ligand and Complexes:

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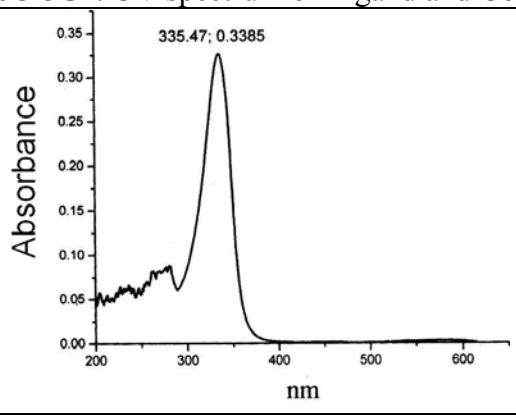
<td> 
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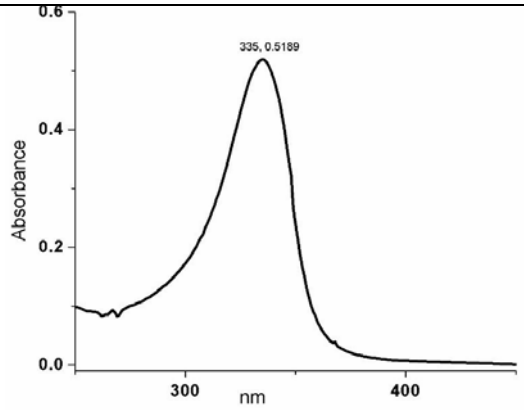
<td> 
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<tr>
<td>(a) Ligand 5 in MeOH; λ_{max} 335 nm, (ε: 1.42 X 10^7 cm^2 mol^{-1}).</td>
<td>(b) Complex 6 in MeOH λ_{max} 335 nm (ε: 6.06 x 10^4 cm^2 mol^{-1})</td>
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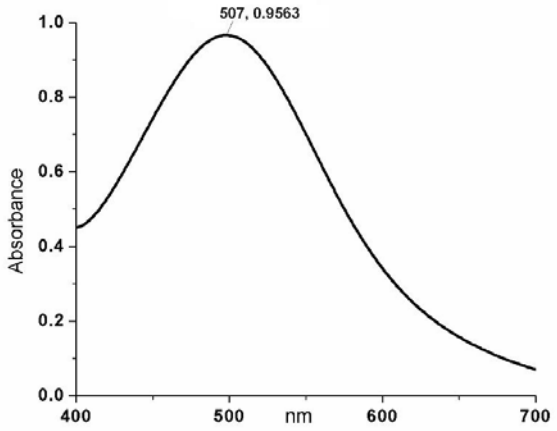
<td> 
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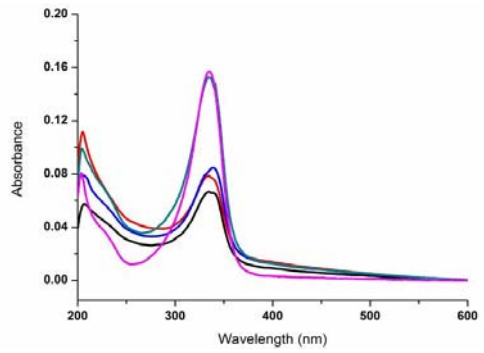
<td> 
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<td>(c) Complex 6 in MeOH λ_{max} 507 nm, (ε: 2.26 X 10^3 cm^2 mol^{-1}).</td>
<td>(d) Complexes in MeOH solution.
7; λ_{max} 336 nm, (ε: 7.50 x 10^4 cm^2 mol^{-1}),
8; λ_{max} 335 nm, (ε: 8.04 X 10^4 cm^2 mol^{-1}),
11; λ_{max} 334 nm, (ε: 2.19 X 10^6 cm^2 mol^{-1}),
12; λ_{max} 334 nm, (ε: 7.80 X 10^4 cm^2 mol^{-1}),
14; λ_{max} 335 nm, (ε: 1.79 X 10^5 cm^2 mol^{-1}).</td>
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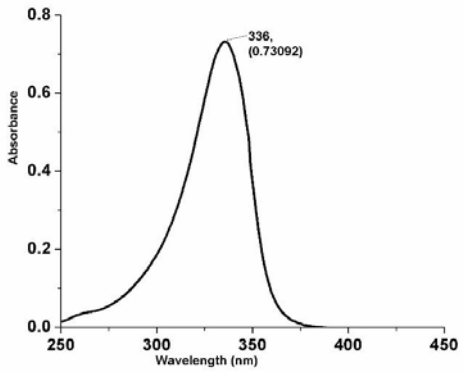
<td> 
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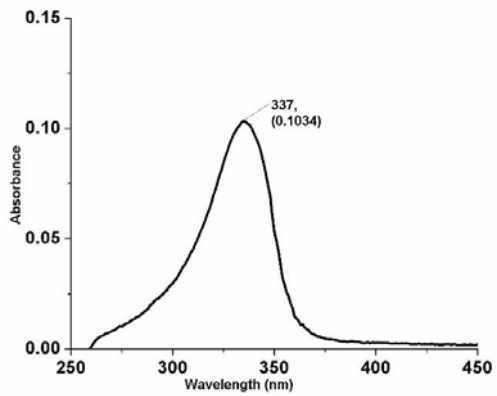
<td> 
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<tr>
<td>(c) Complex 9 in MeOH
λ_{max} 336 nm, (ε: 5.375 x 10^4 cm^2 mol^{-1})</td>
<td>(c) Complex 10 in MeOH
λ_{max} 337 nm, (ε: 8.510 x 10^3 cm^2 mol^{-1})</td>
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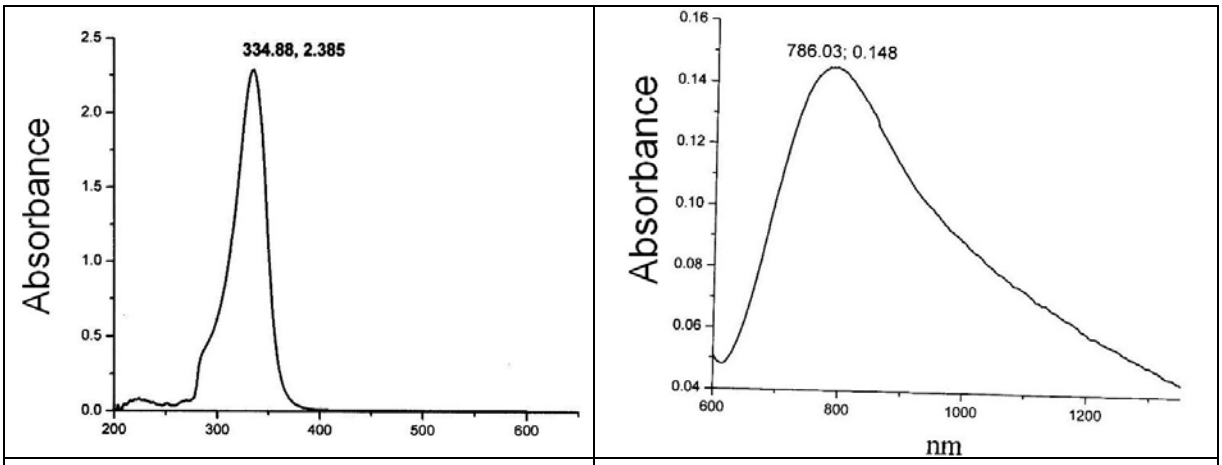
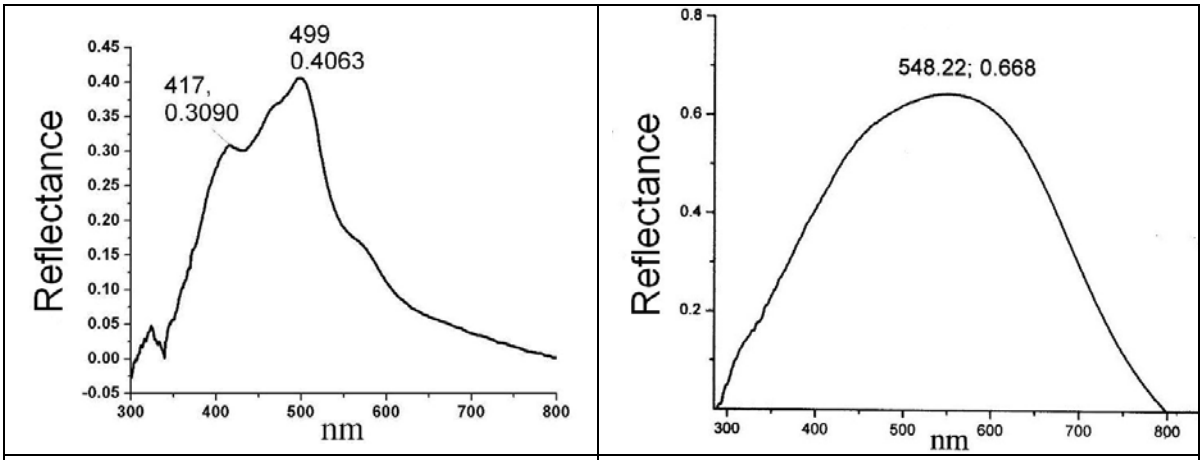


(e) Complex **13** in MeOH λ_{max} 335 nm (ε: 5.59x10^4 cm^2 mol^{-1})

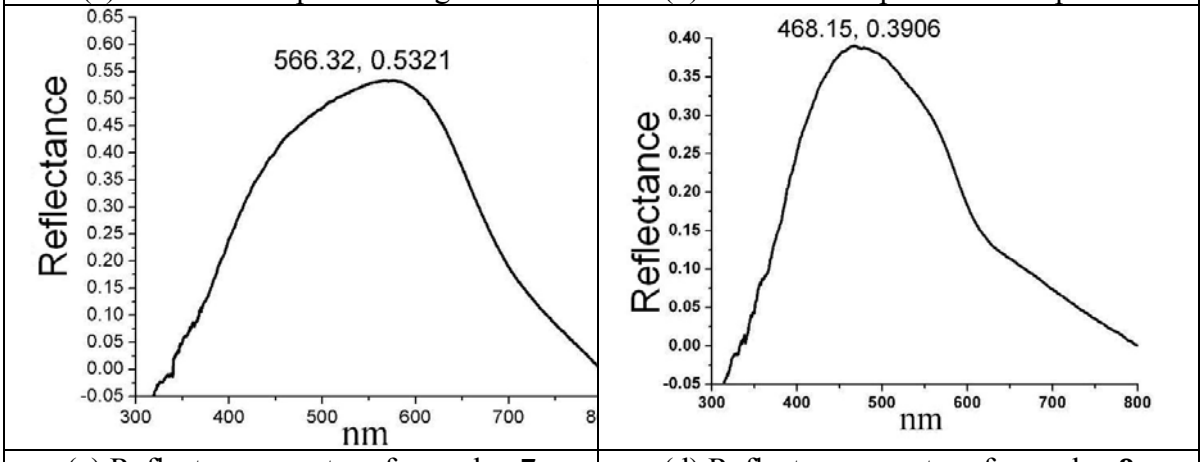
(f) Complex **13** in MeOH, λ_{max} 786 nm (ε: 34.66 cm^2 mol^{-1})

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



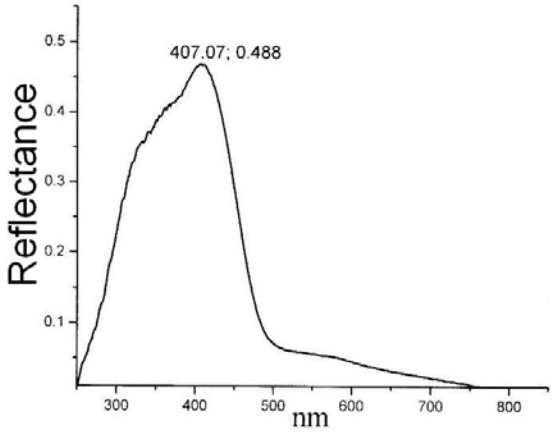
(a) Reflectance spectra of ligand **5**

(b) Reflectance spectra of complex **6**

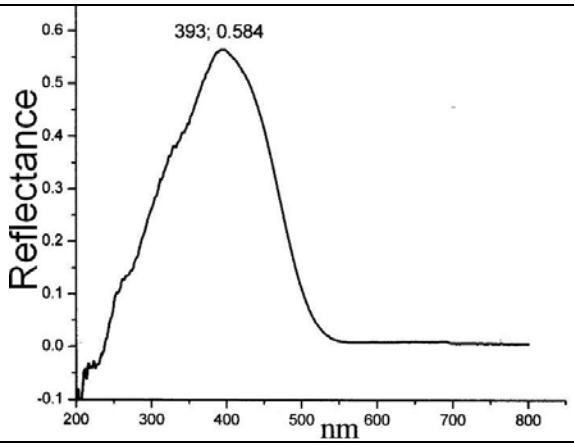


(c) Reflectance spectra of complex **7**

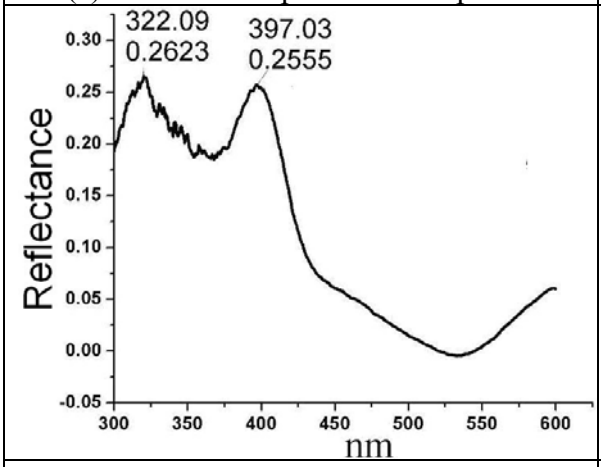
(d) Reflectance spectra of complex **8**



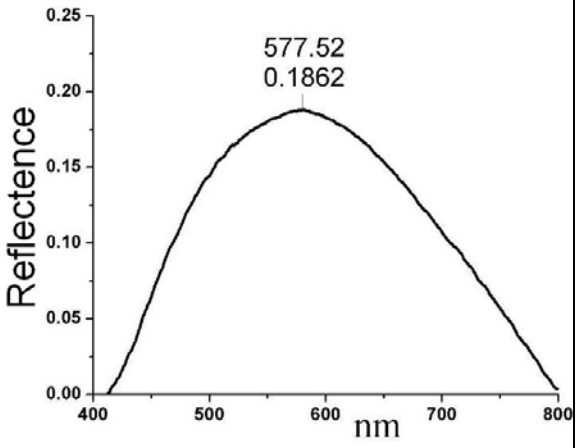
(e) Reflectance spectra of complex **9**



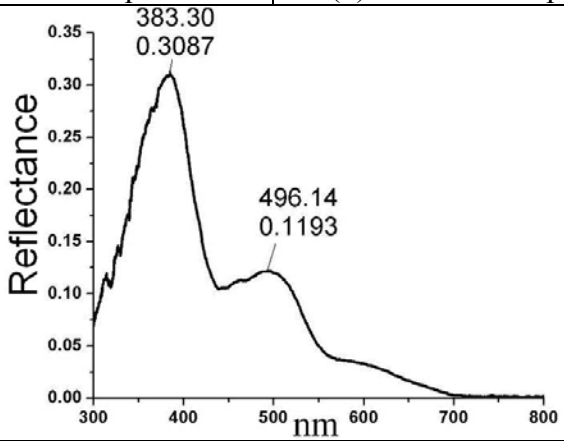
(f) Reflectance spectra of complex **10**



(g) Reflectance spectra of complex **11**



(h) Reflectance spectra of complex **12**



(I) Reflectance spectra of complex **14**

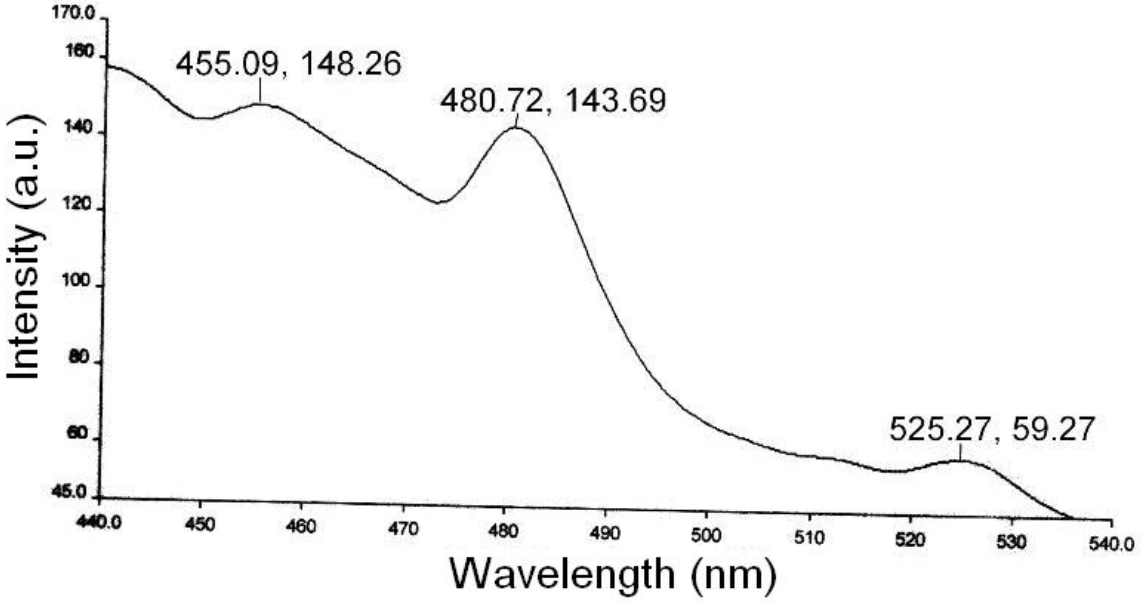


Figure S8. Emission Spectra of Complexes **9**.

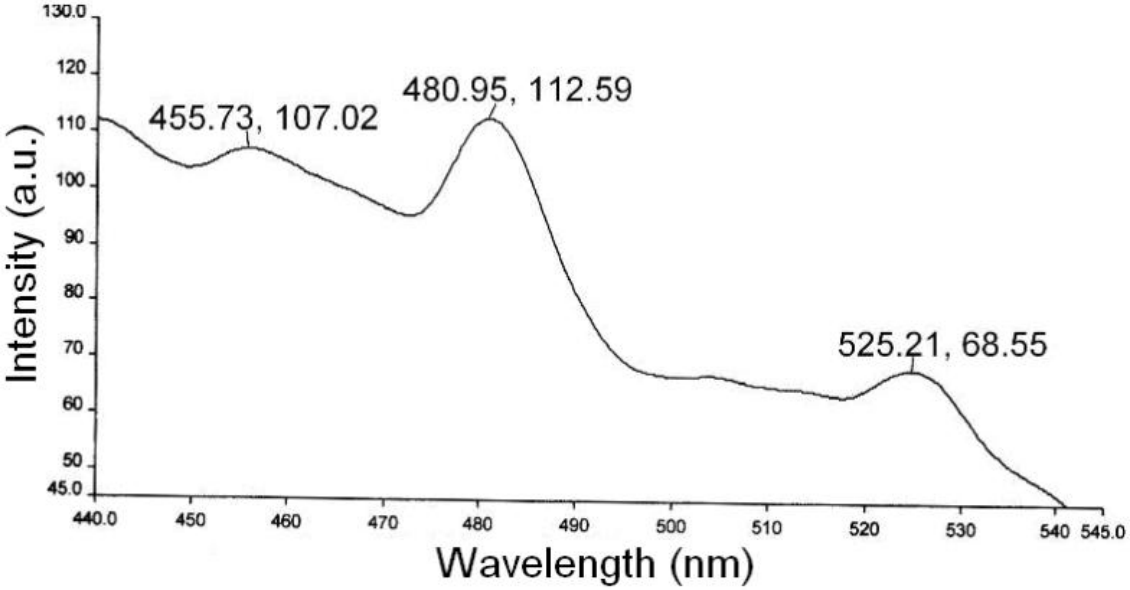


Figure S9. Emission Spectra of Complexes **10**.

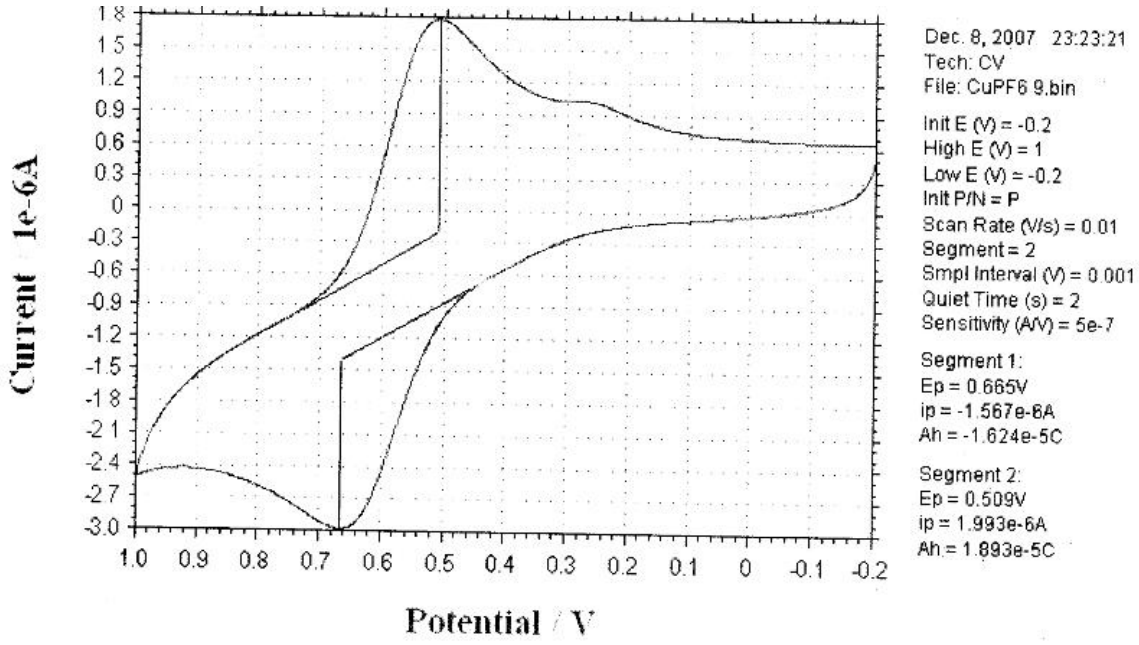


Figure S10. Cyclic Voltammogram of **6**.

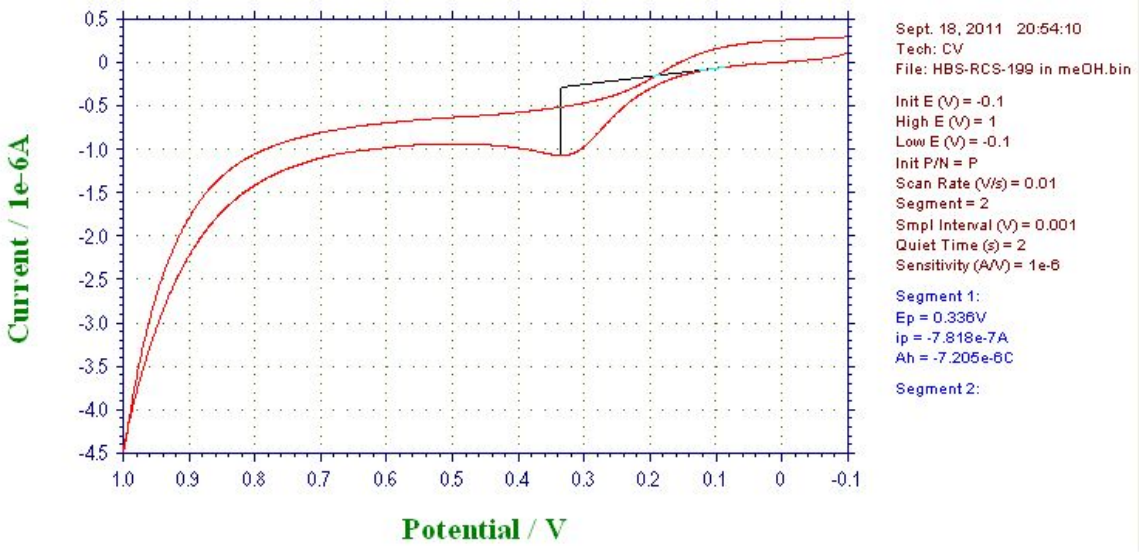


Figure S11. Cyclic Voltammogram of **8.**

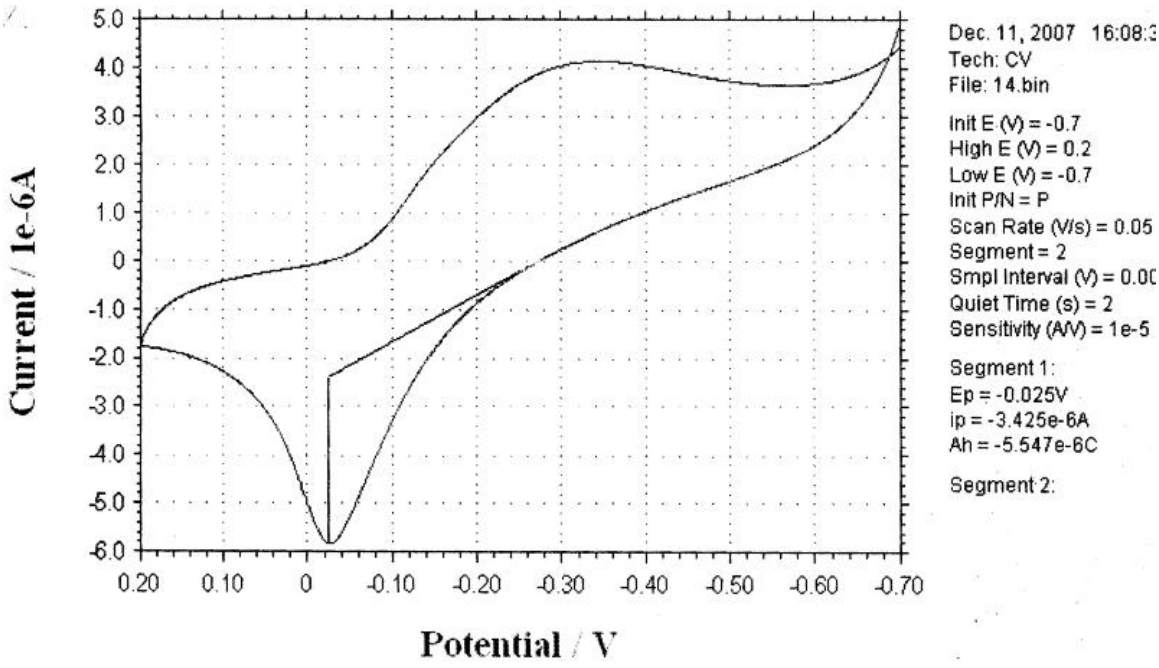


Figure S12. Cyclic Voltammogram of **13**.

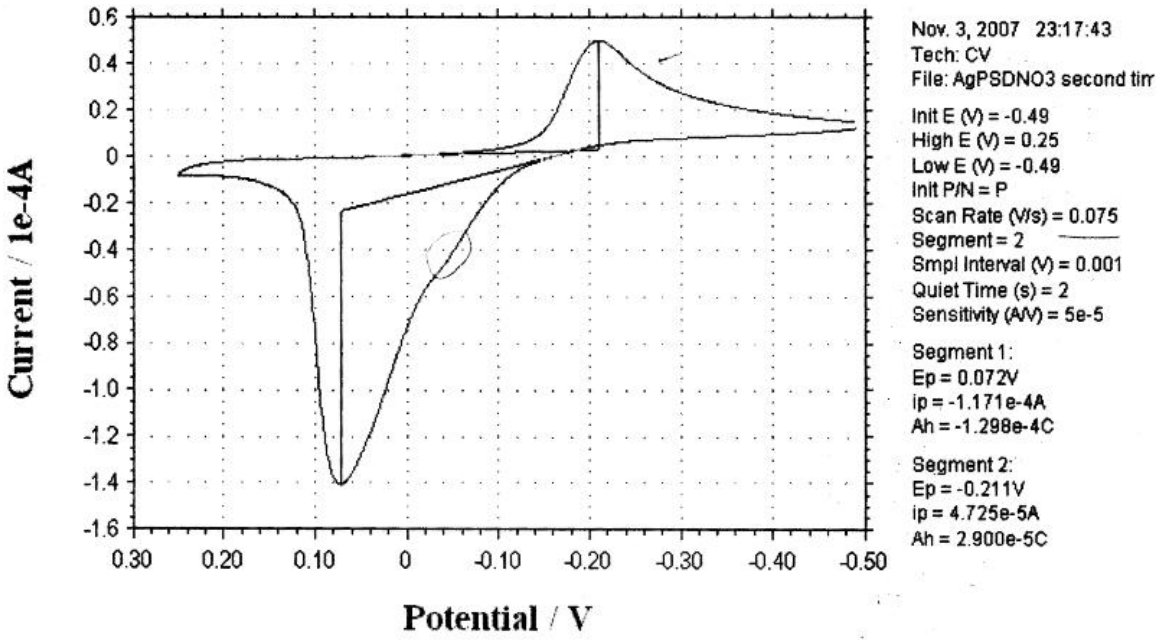


Figure S13. Cyclic Voltammogram of **9.**

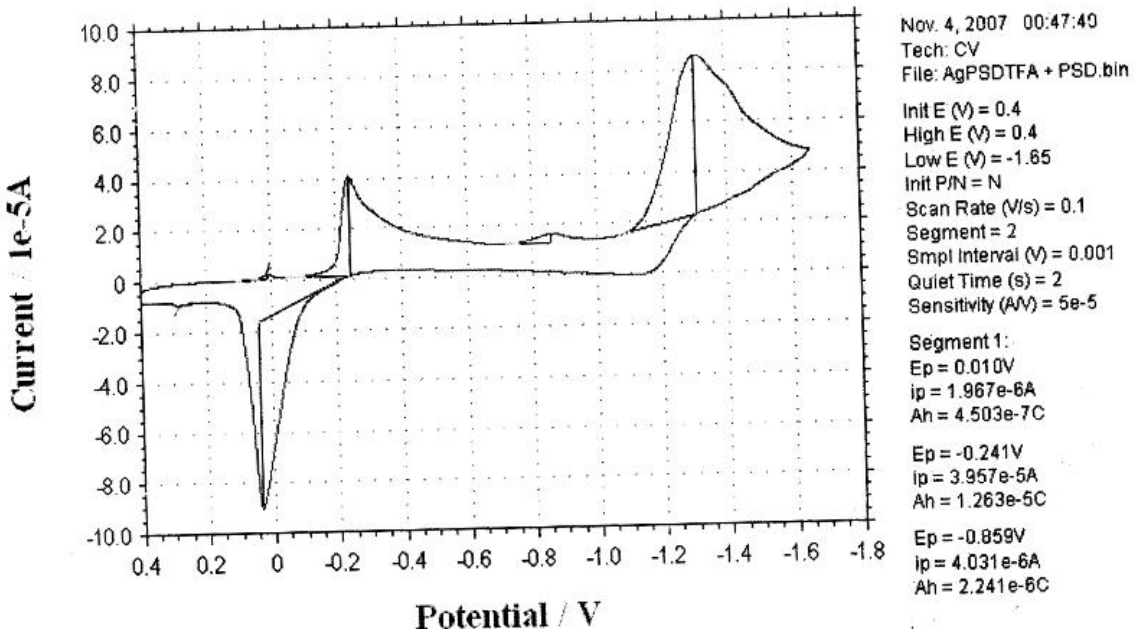
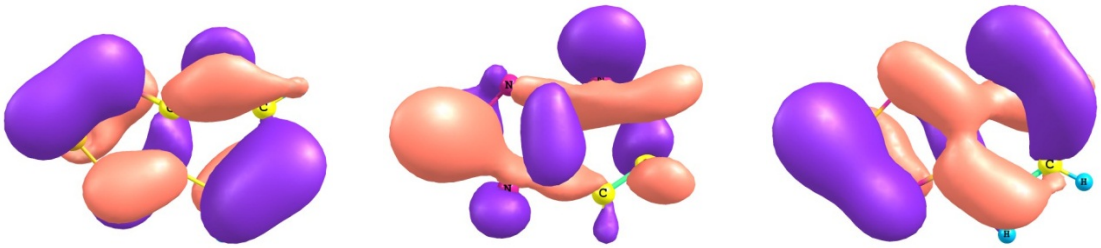


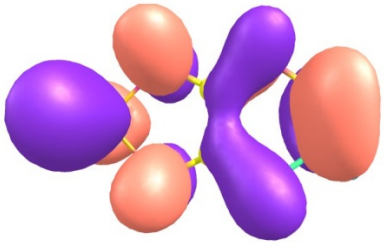
Figure S14. Cyclic Voltammogram of **10**.

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

Compound 5:λ = 288 nm (*f* = 0.234);
The major contributing MO's are as follows
HOMO−2→LUMO ;HOMO−1→LUMO ; HOMO→LUMO

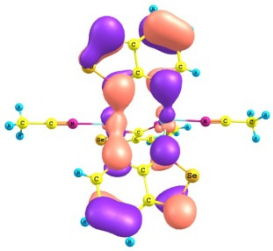


HOMO-2 HOMO-1 HOMO

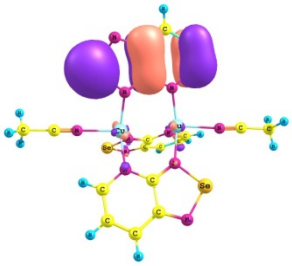


LUMO

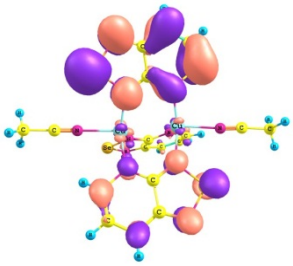
Compound 6: λ = 296 nm (*f* = 0.138); 549 nm (*f* = 0.040),
For transition at 296 nm, the major contributing MO's are shown below:
HOMO−15→LUMO+2; HOMO−13→LUMO+1



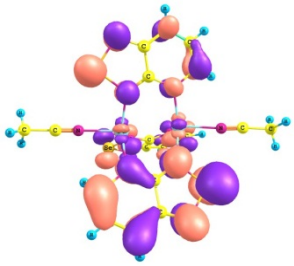
HOMO−15



HOMO−13



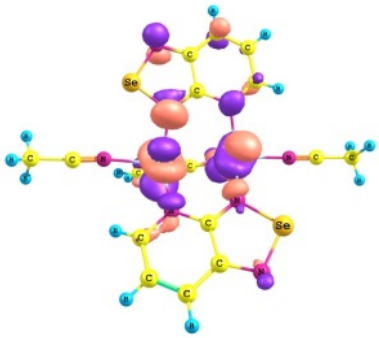
LUMO+1



LUMO+2

For transition at 547 nm, the major contributing MO's are:

HOMO−3→LUMO+1 ; HOMO−3→LUMO+2

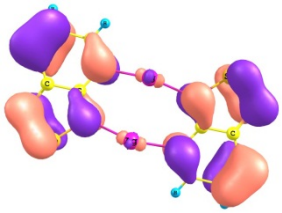


Compound 9: λ = 295 nm (*f* = 0.312);

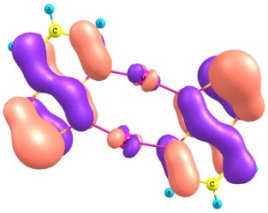
The major contributing MO's are shown below:

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

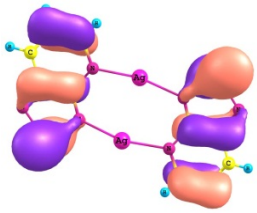
HOMO→LUMO



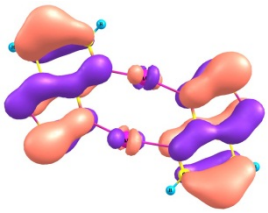
HOMO–4



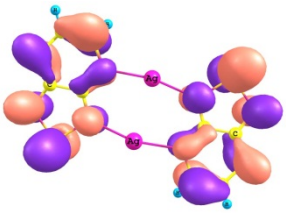
HOMO–2



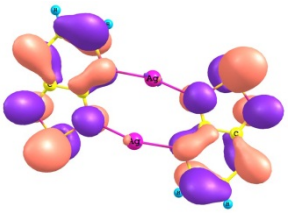
HOMO–1



HOMO



LUMO

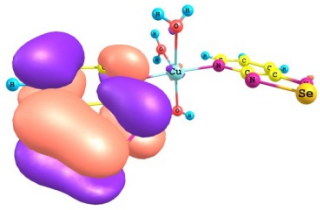


LUMO+1

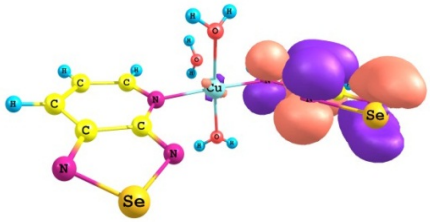
Compound 13: λ = 293 nm (*f* = 0.321); and 786 nm (*f* = 0.0001);

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

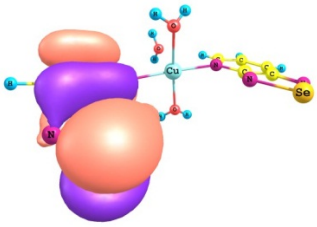
(HOMO–3)α→(LUMO)α; (HOMO–2)α→(LUMO+1)α; (HOMO-1)α→(LUMO)α; (HOMO)α→(LUMO+1)α; (HOMO–2)β→(LUMO+2)β; (HOMO-1)β→(LUMO+1)β; (HOMO)β→(LUMO+2)β;



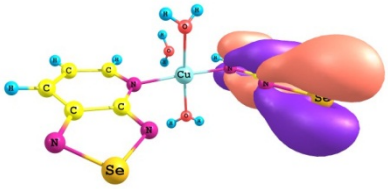
(HOMO–3)α



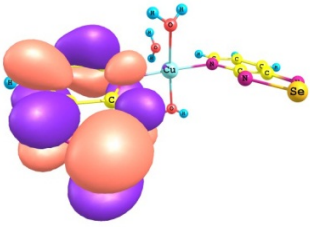
(HOMO–2)α



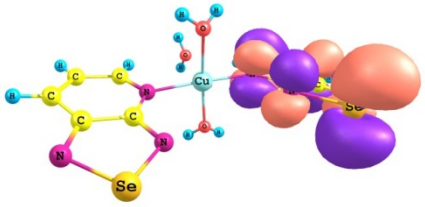
(HOMO–1)α



(HOMO)α

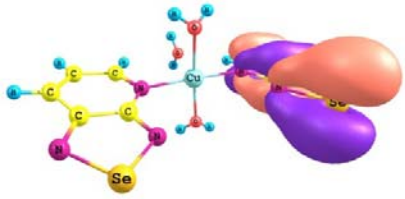


(LUMO)α

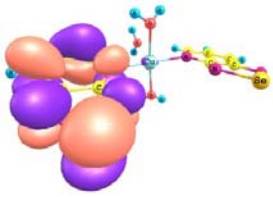


(LUMO+1)α

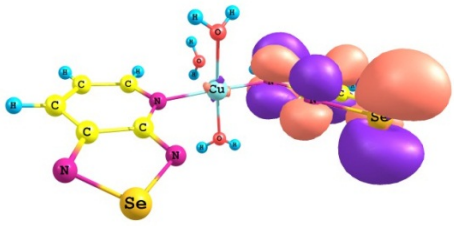
(HOMO–2)β



(HOMO)β



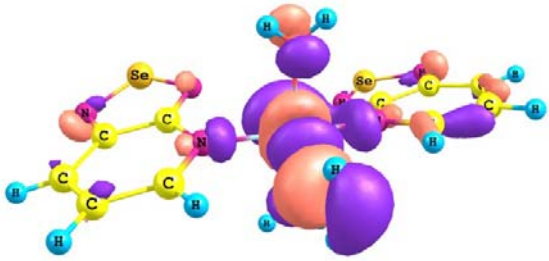
(LUMO+1)β



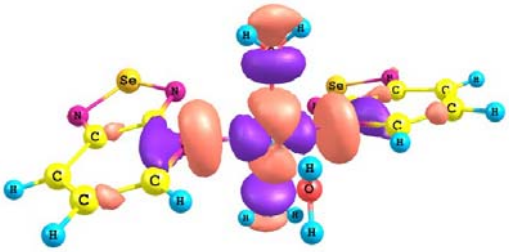
(LUMO+2)β

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

(HOMO−10)β→(LUMO)β



(HOMO−10)β



(LUMO)β

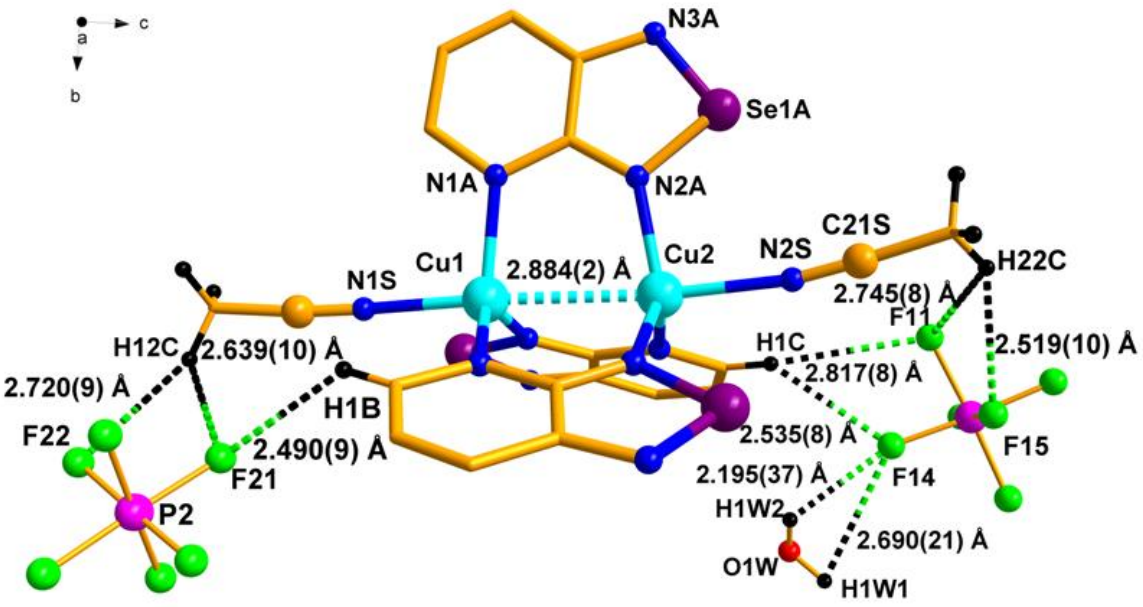


Figure S15. 1-D Supramolecular motif via C─H···F and H···F hydrogen bonding in the lattices of **6**. Only relevant hydrogen atoms are shown for clarity.

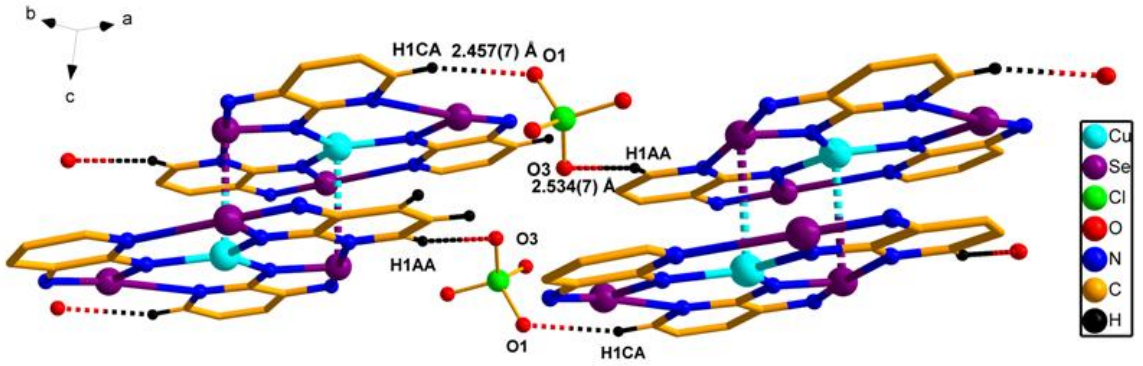
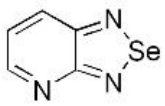


Figure S16. 1-DSupramolecular motif via C─H···O hydrogen bonding in the lattices of **8**. Only relevant hydrogen atoms are shown for clarity.

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
Analysed : 03/26/2007 14:54
Sample ID : HBS-GM-PSD (# 23)
Analysis Type : UnkNown (Area)

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

$[Cu_2(psd)_3(CH_3CN)_2]\,2PF_6$

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

Method Name : sp210807
Method File : G:\eager300\Eager 300 EA1112\SP210807.mth
Chromatogram : GMCU-I
Operator ID : sp
Analysed : 08/21/2007 13:28
Sample ID : GMCU-I (# 15)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 8/21/2007 16:31
Instrument N. : Instrument #1
Sample weight : 1.703

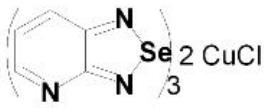
Calib. method : using 'K Factors'

!!! 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
Analysed : 03/04/2010 13:03
Sample ID : CG-A-19-10 (# 17)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 3/4/2010 14:57
Instrument N. : Instrument #1
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

$[Cu_2(psd)_6]\ 2ClO_4$

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

Method Name : SP010410
Method File : D:\CHNS2008\SP010410.mth
Chromatogram : CG-A-19-15
Operator ID : MP
Analysed : 04/01/2010 12:24
Sample ID : CG-A-19-15 (# 10)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 4/1/2010 15:19
Instrument N. : Instrument #1
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

$[Ag_2(psd)_2]\ 2NO_3$

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

$[Ag_2(psd)_2]\ 2CF_3COOO$

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

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 $[Cu(psd)_4(H_2O)_3]\ 2ClO_4$

Page: 1 Sample: CGA19-4 (CGA19-4)

Method Name : SP290110
Method File : D:\CHNS2008\SP290110.mth
Chromatogram : CGA19-4
Operator ID : SP
Analysed : 01/29/2010 15:10
Sample ID : CGA19-4 (# 30)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 1/29/2010 16:35
Instrument N. : Instrument #1
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 $[Cu(psd)_4(H_2O)]\ 2ClO_4(CHCl_3)$

Page: 1 Sample: CGA19-5-2 (CGA19-5-2)

Method Name : SP290110
Method File : D:\CHNS2008\SP290110.mth
Chromatogram : CGA19-5-2
Operator ID : SP
Analysed : 01/29/2010 13:12
Sample ID : CGA19-5-2 (# 19)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 1/29/2010 16:32
Instrument N. : Instrument #1
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

$[Cu(psd)_4(H_2O)_4]\ 2NO_3$

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

[Co(psd)4(H2O)4] (ClO4)2

Page: 1 Sample: RCS-303 (RCS-303)

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.**

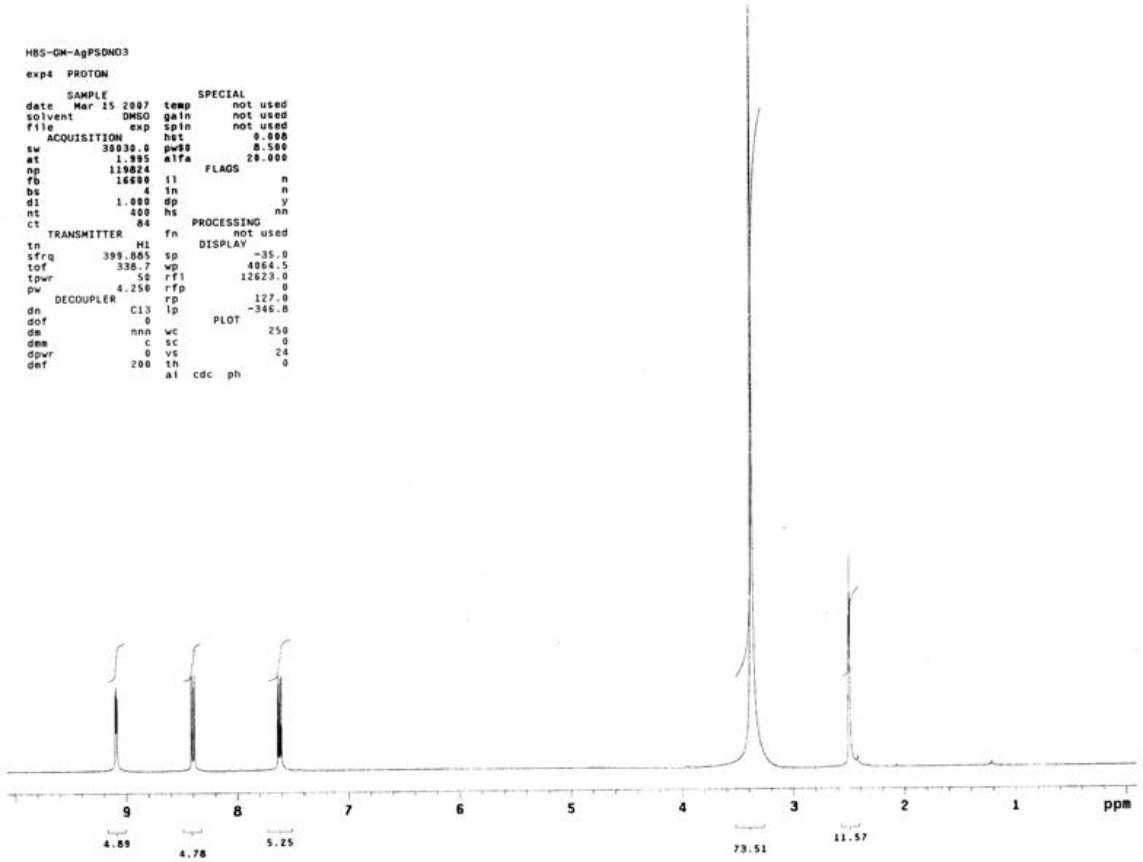


Figure S27. ^{1}H NMR spectrum of **9** in DMSO-d_6.

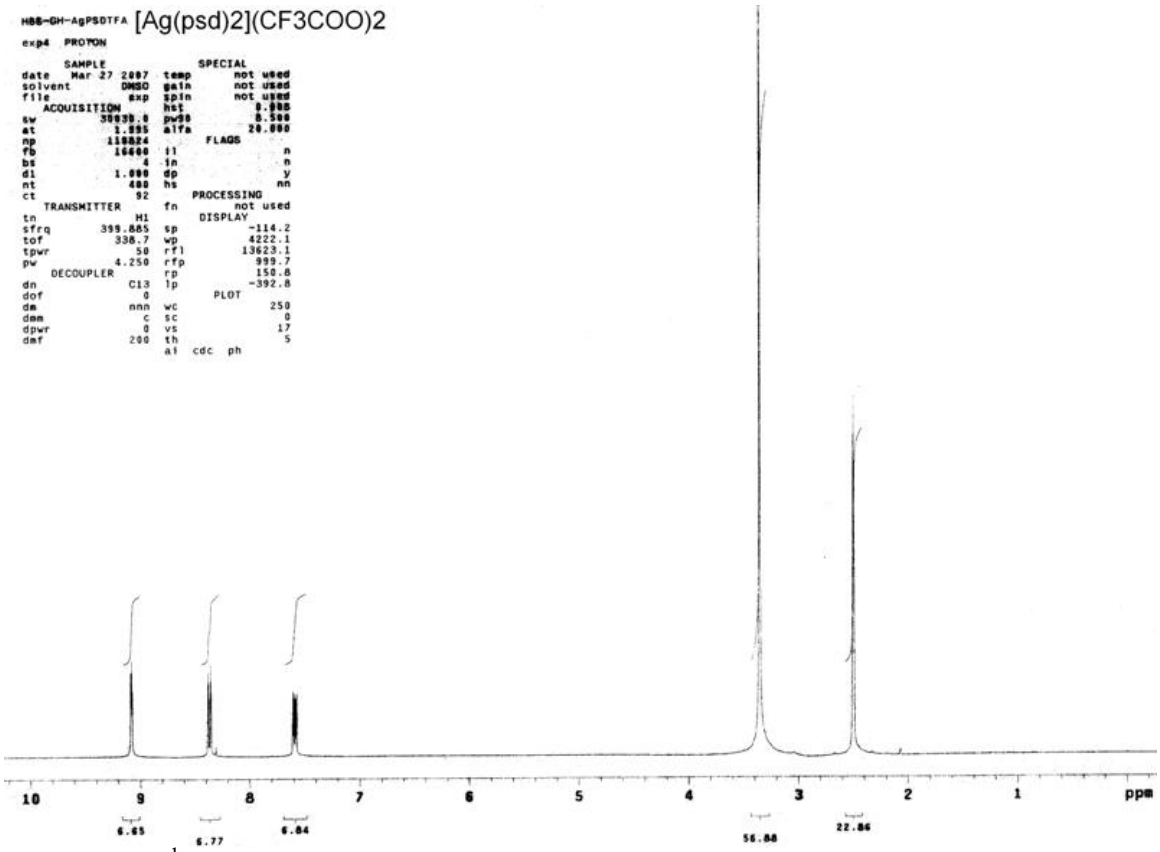


Figure S28. ^{1}H NMR spectrum of **10** in DMSO-d_6.

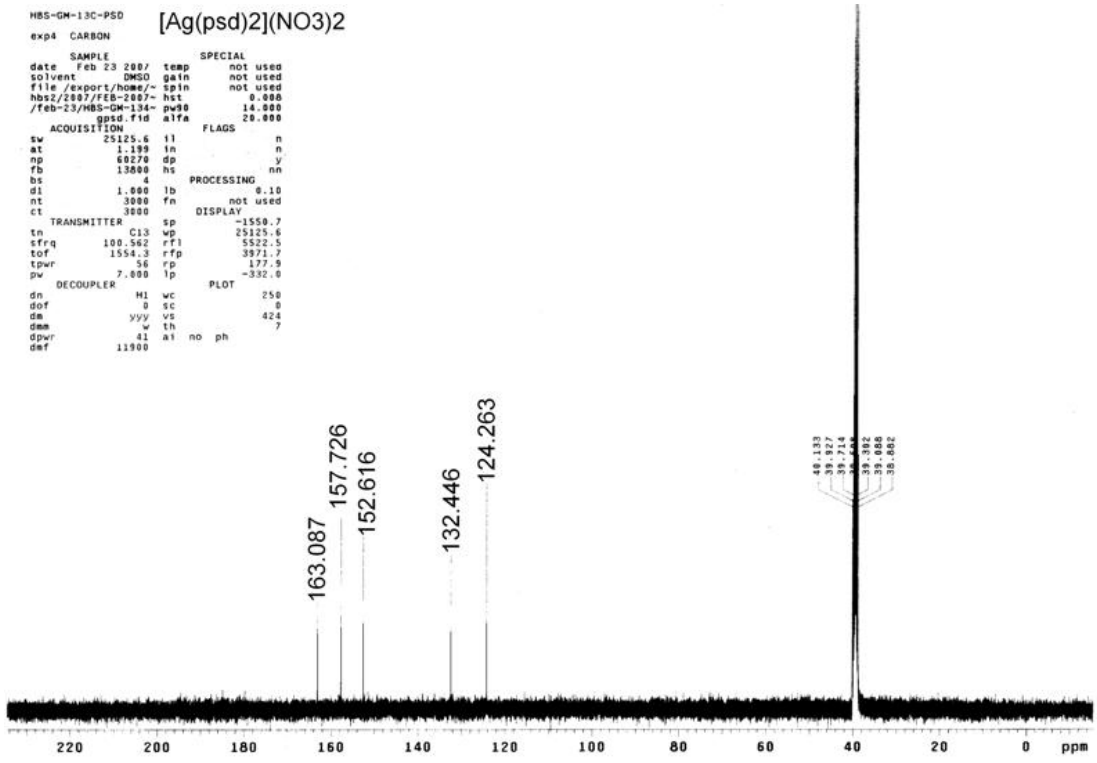


Figure S29. ^{13}C NMR spectrum of **9** in DMSO-d_6.

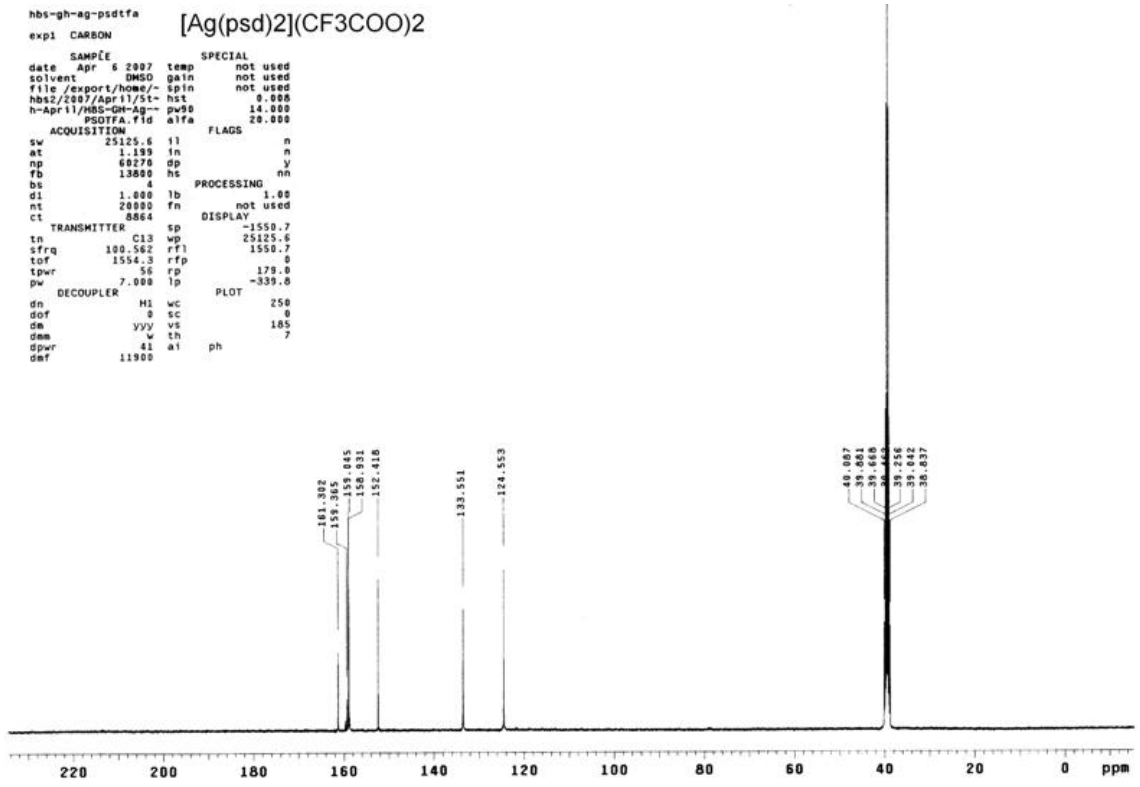


Figure S30. ^{13}C NMR spectrum of **10** in DMSO-d_6.

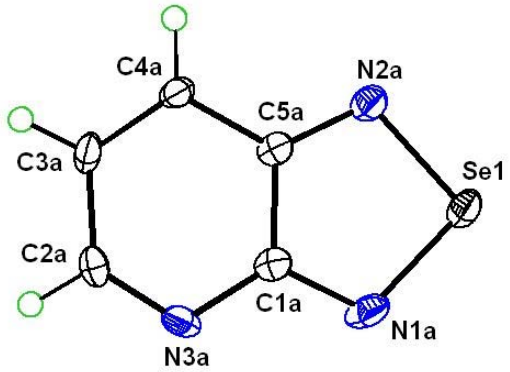


Figure S31. ORTEP diagram of **5**.

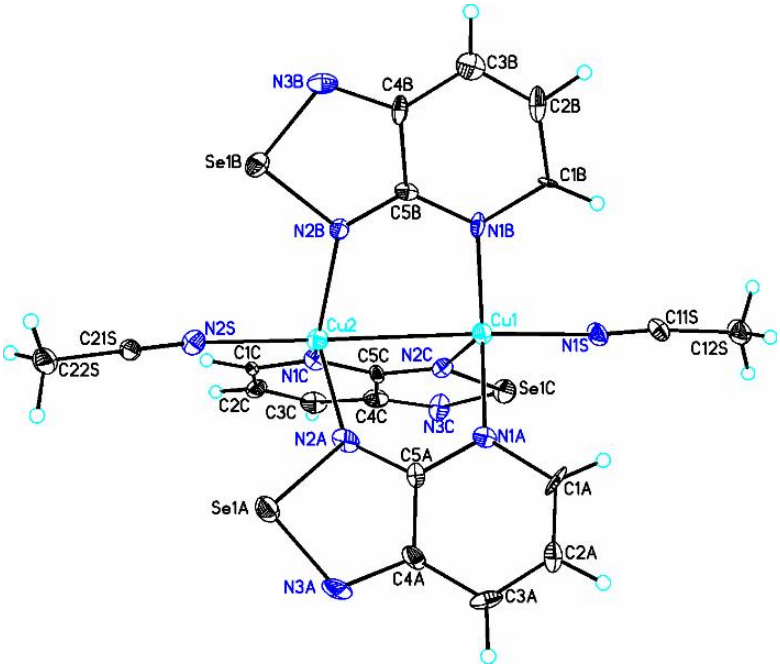


Figure S32. ORTEP diagram of the cationic part of **6**.

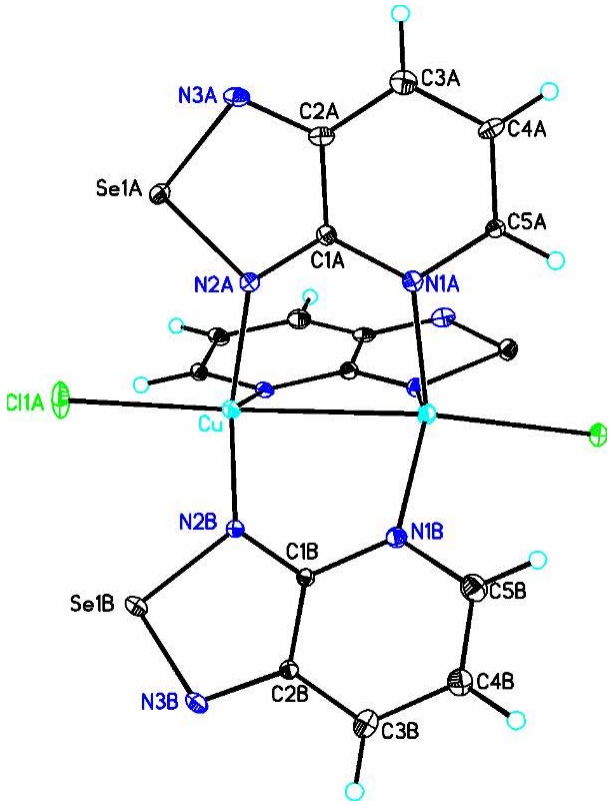


Figure S33. ORTEP diagram of the **7**.

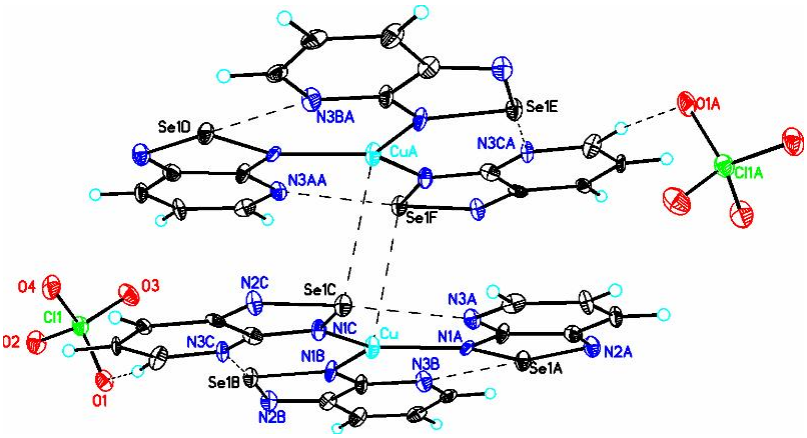


Figure S34. ORTEP diagram of **8**.

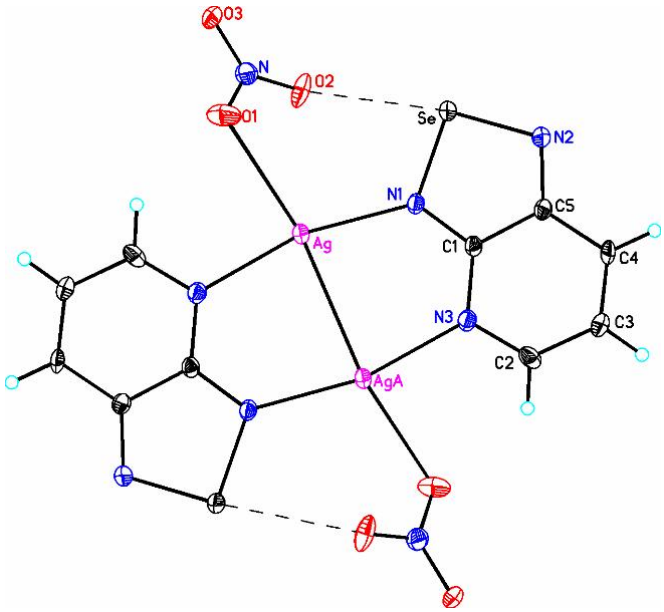


Figure S35. ORTEP diagram of **9**.

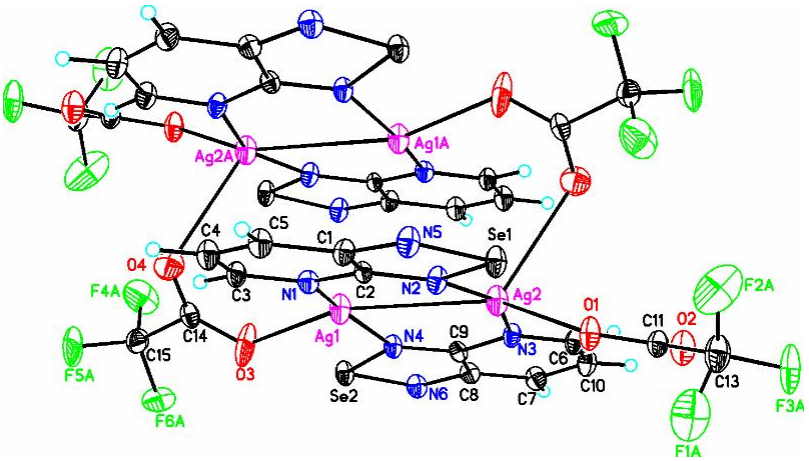


Figure S36. ORTEP diagram of **10**.

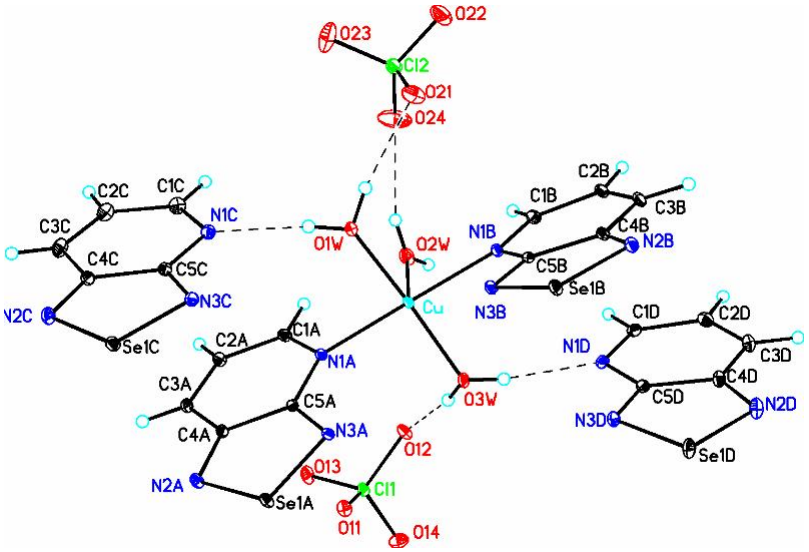


Figure S37. ORTEP diagram of **11**.

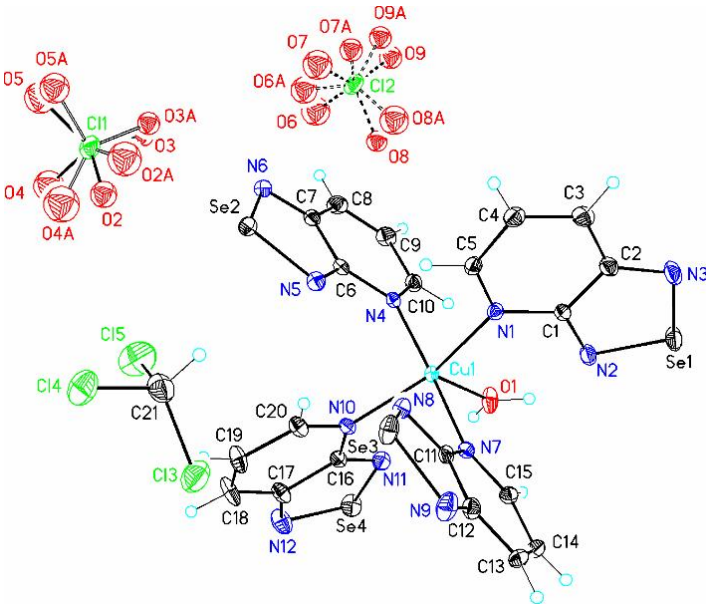


Figure S38. ORTEP diagram of **12**.

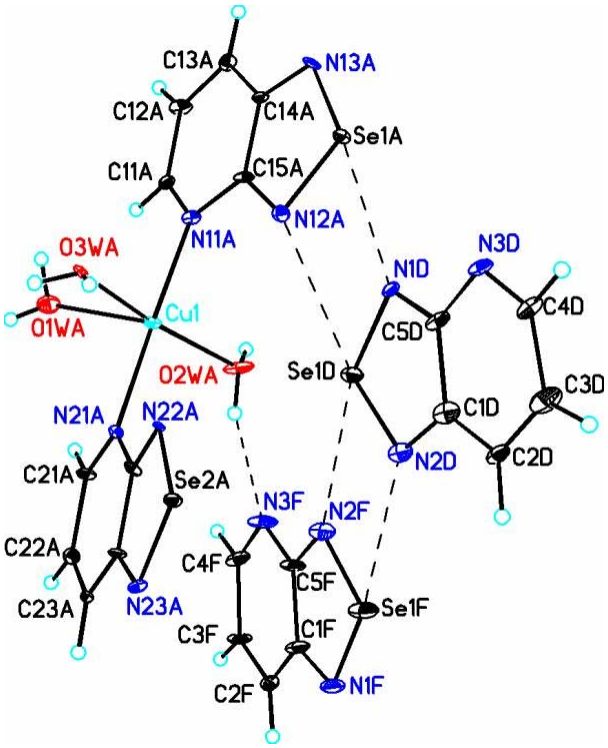


Figure S39. ORTEP diagram of the cationic part of **13**. Selected bond distances [Å] and angles [º]: Cu(2)–N(11B) 2.038(5), Cu(2)–N(21B) 2.060(5), Cu(2)–O(1WB) 2.259(4), Cu(2)–O(2WB) 1.956(3), Cu(2)–O(3WB) 1.927(3), Se(2B)•••N(1C) 2.877(5), Se(1C)•••N(2B) 3.031(5), Se(1C)•••N(1E)

3.006(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).

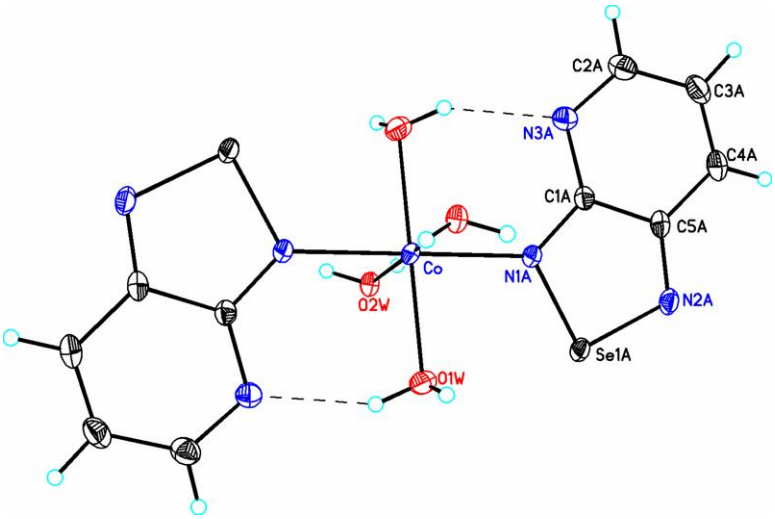


Figure S40. ORTEP diagram **o**f the cationic part of **14**.

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
6					
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
8					
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
9					
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
10					
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
11					
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)	
12					
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
13					
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	
14					
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