

Supporting Information

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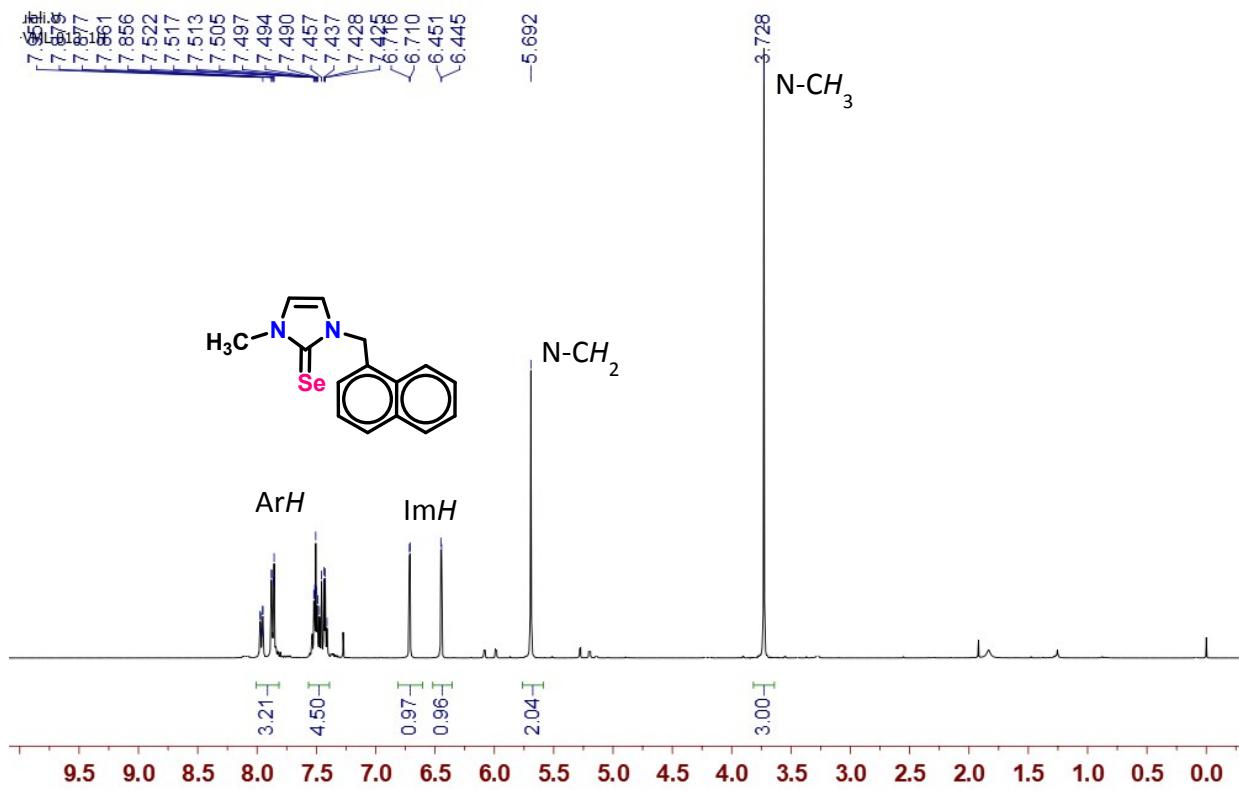


Fig. S 1. ¹H NMR spectrum of **L¹** in CDCl₃

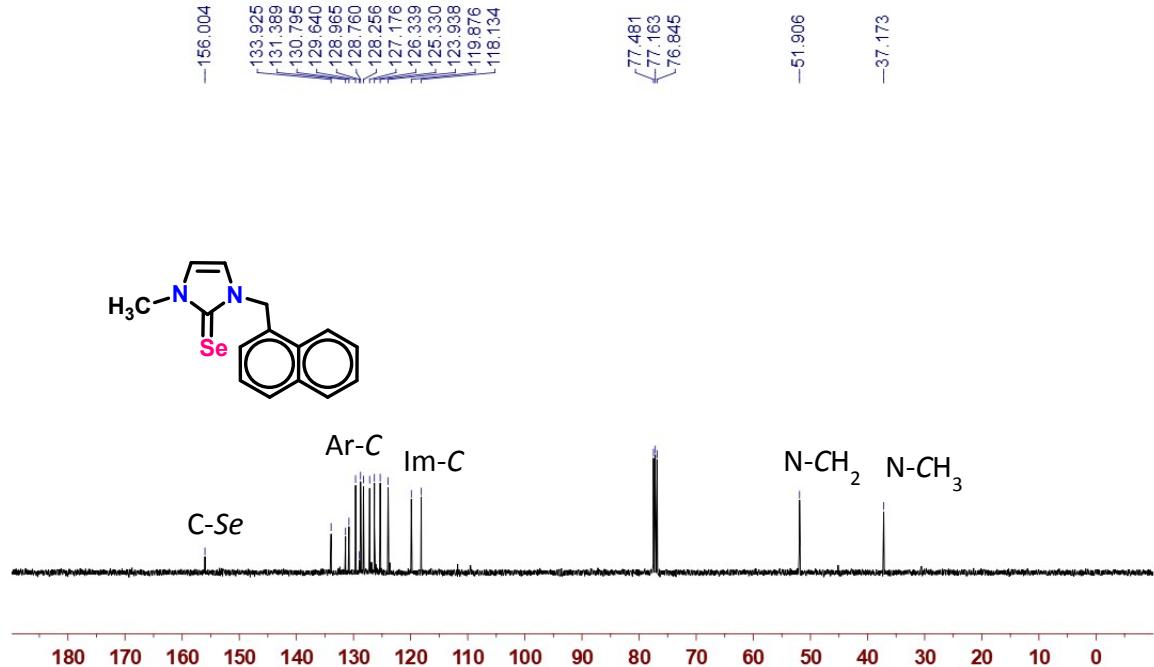


Fig. S 2. ¹³C NMR spectrum of **L¹** in CDCl₃

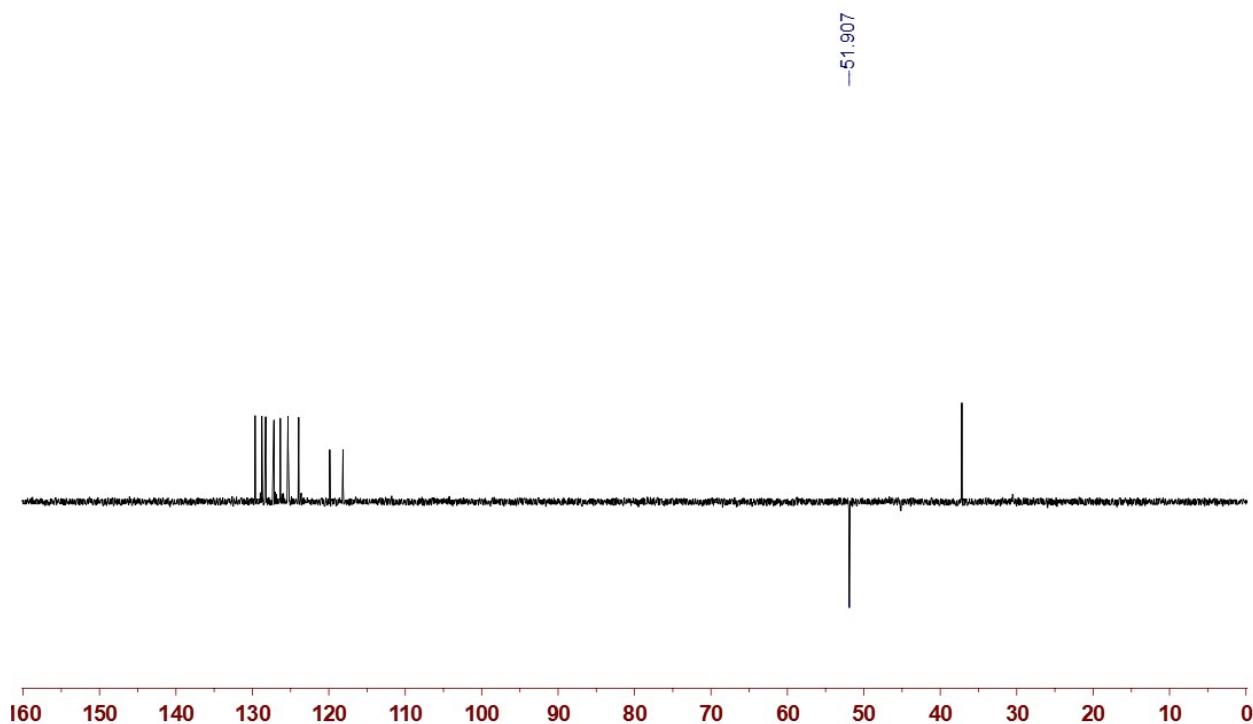


Fig. S 3. DEPT NMR spectrum of **L¹** in CDCl_3

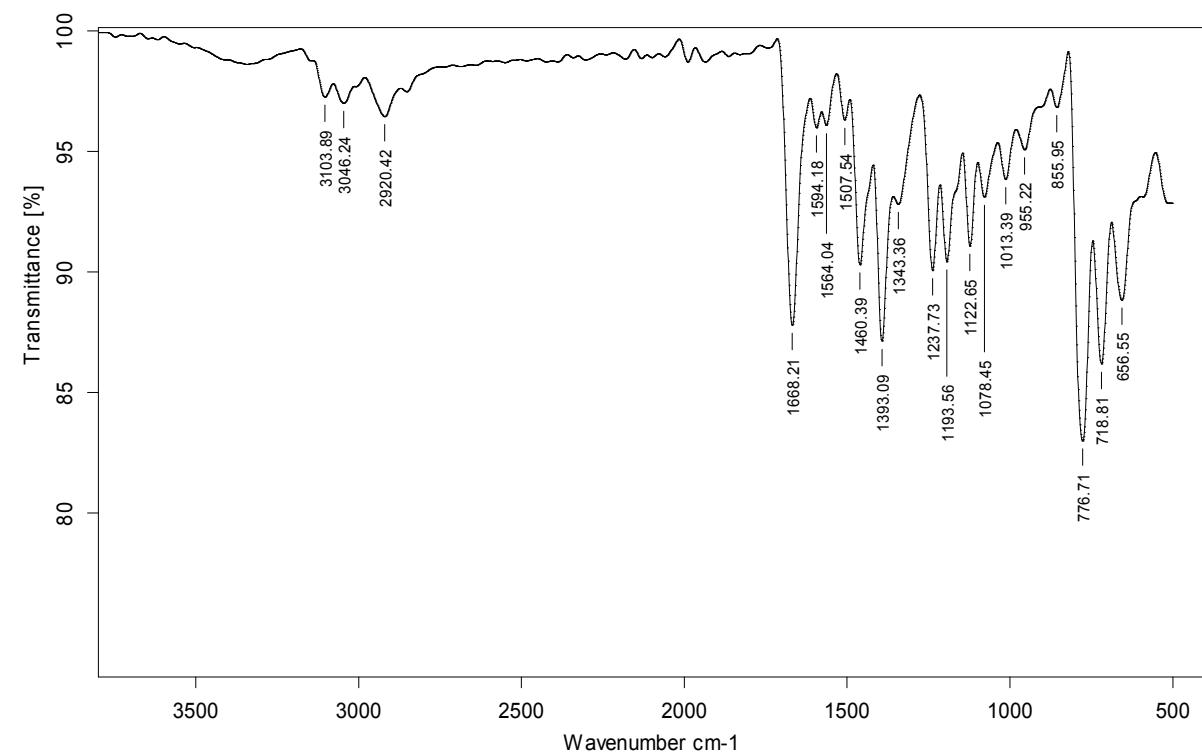


Fig. S 4. Neat FT-IR spectrum of **L¹**.

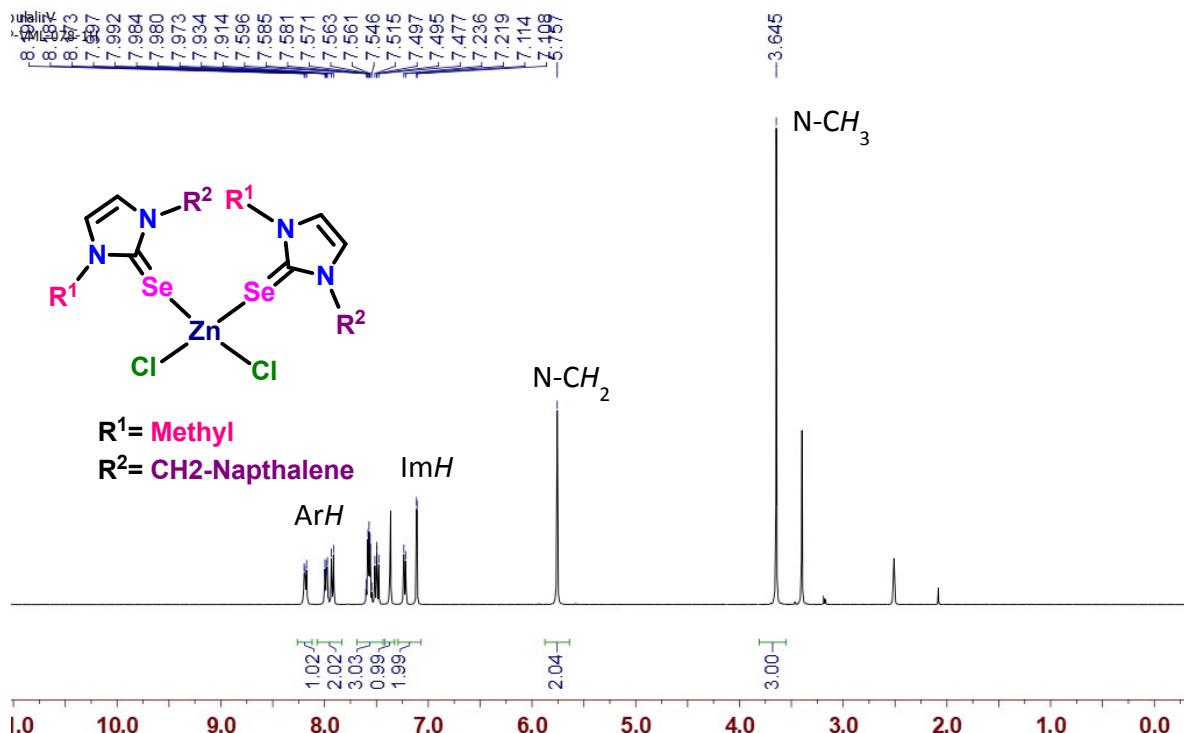


Fig. S 5. ^1H NMR spectrum of complex **1** in $\text{DMSO}-d_6$

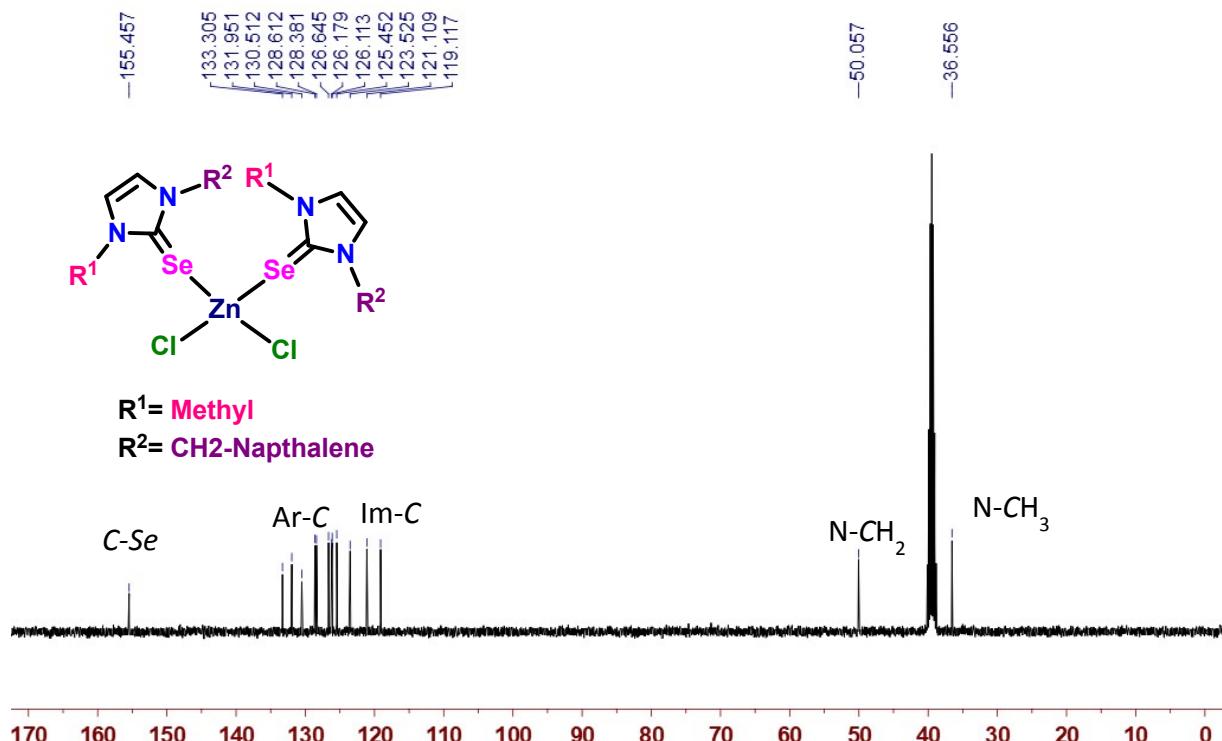


Fig. S 6. ^{13}C NMR spectrum of complex **1** in $\text{DMSO}-d_6$

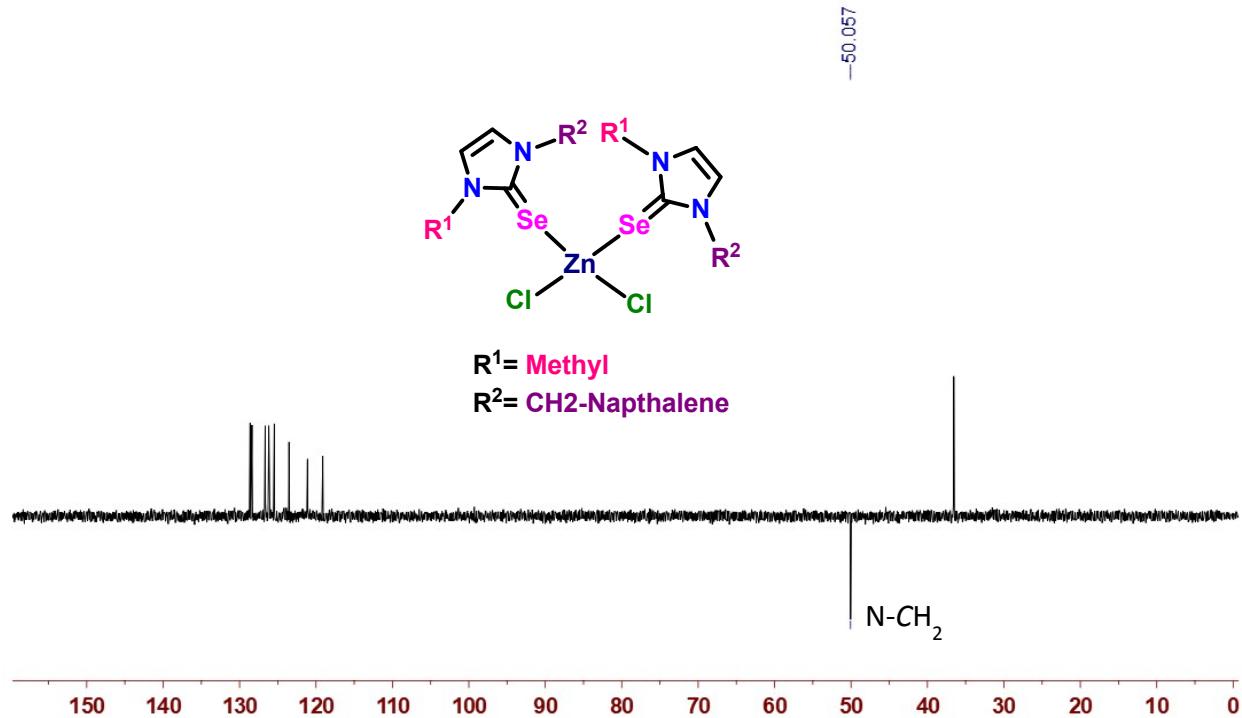


Fig. S 7. DEPT NMR spectrum of complex **1** in $\text{DMSO}-d_6$

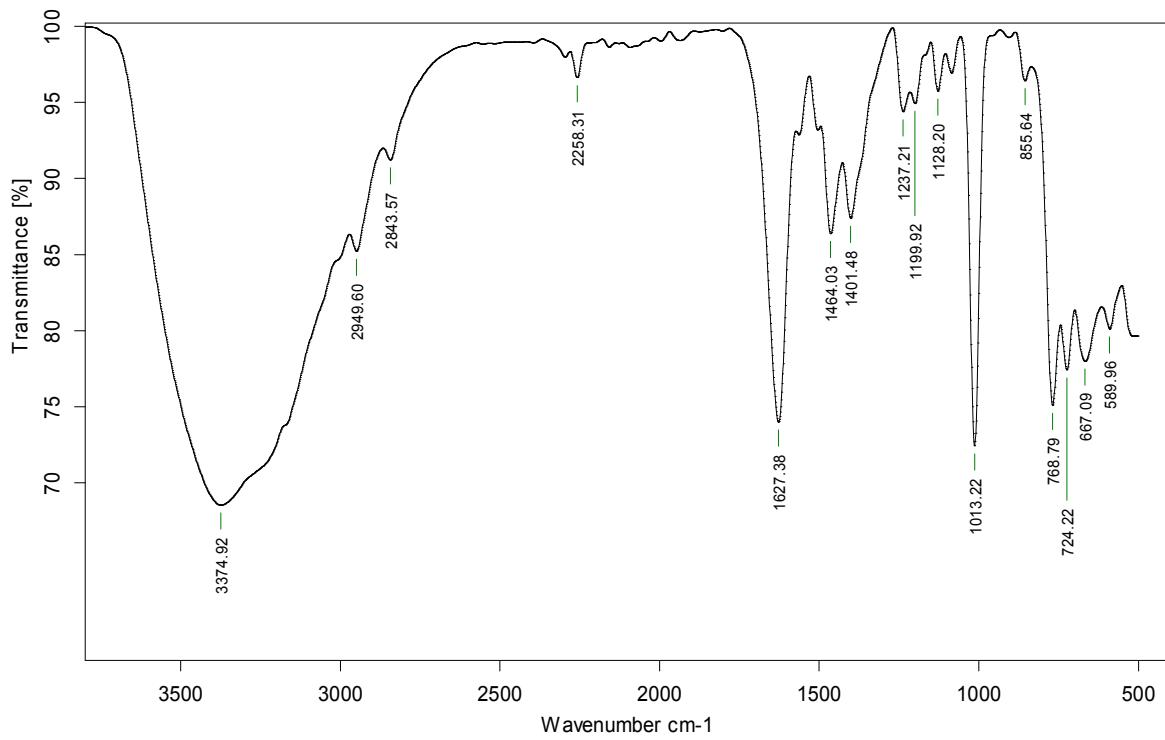


Fig. S 8. Neat FT-IR spectrum of complex

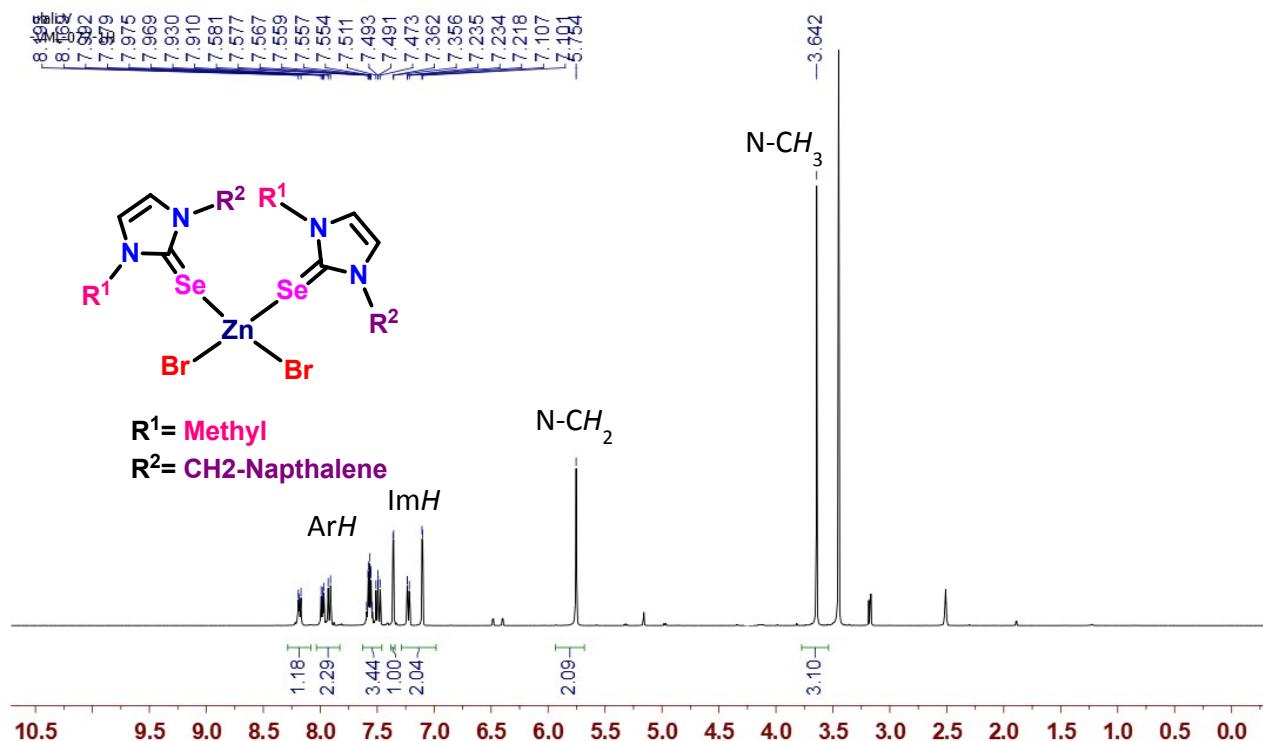


Fig. S 9. ^1H NMR spectrum of complex **2** in $\text{DMSO}-d_6$

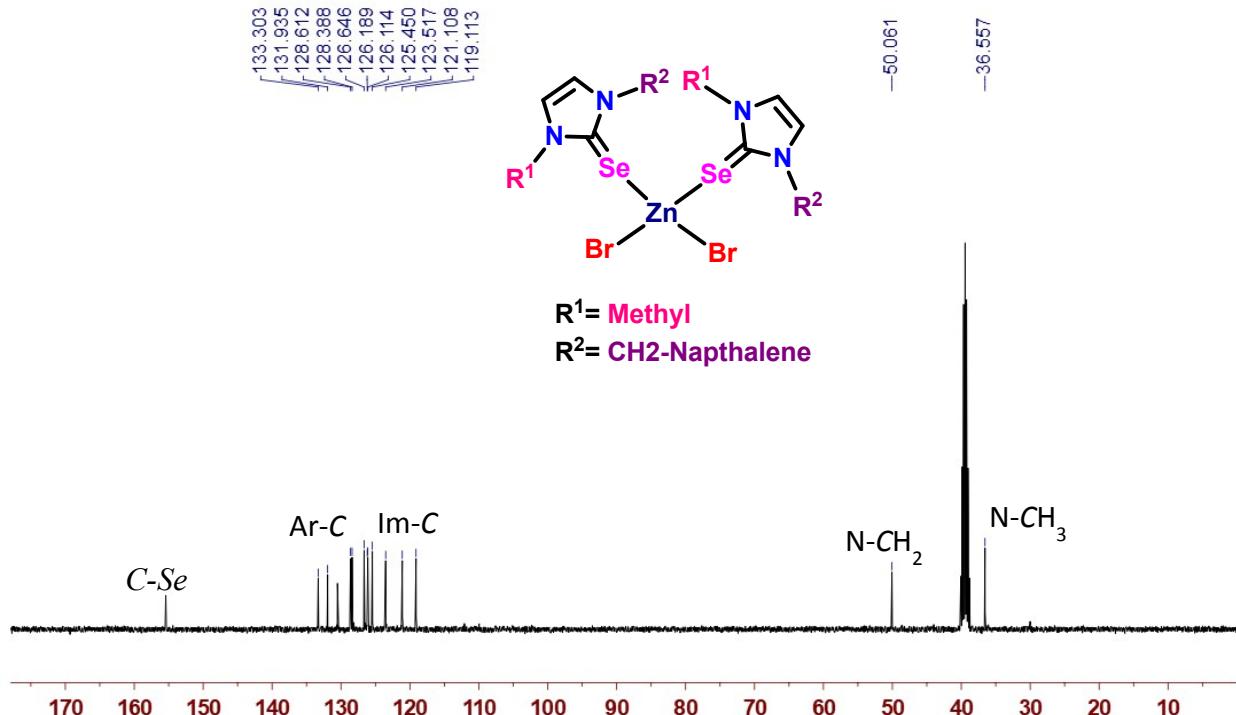


Fig. S10. ^{13}C NMR spectrum of complex **2** in $\text{DMSO}-d_6$

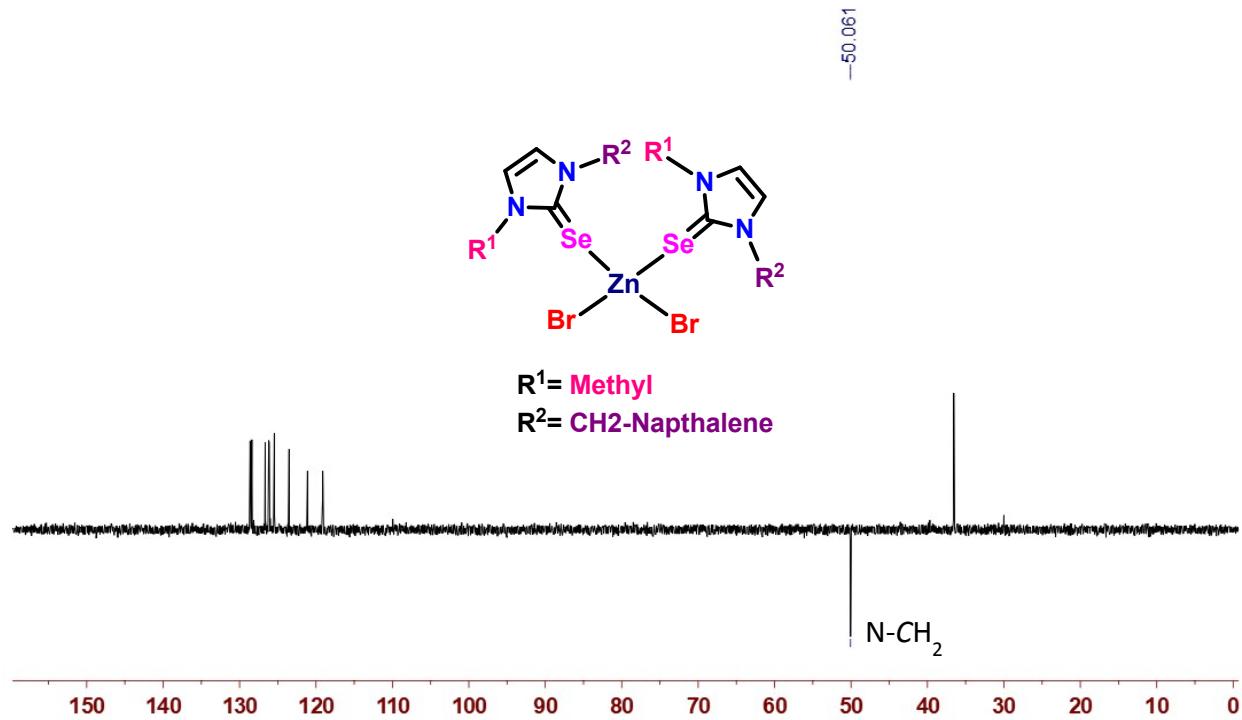


Fig. S11. DEPT NMR spectrum of complex **2** in DMSO-*d*₆

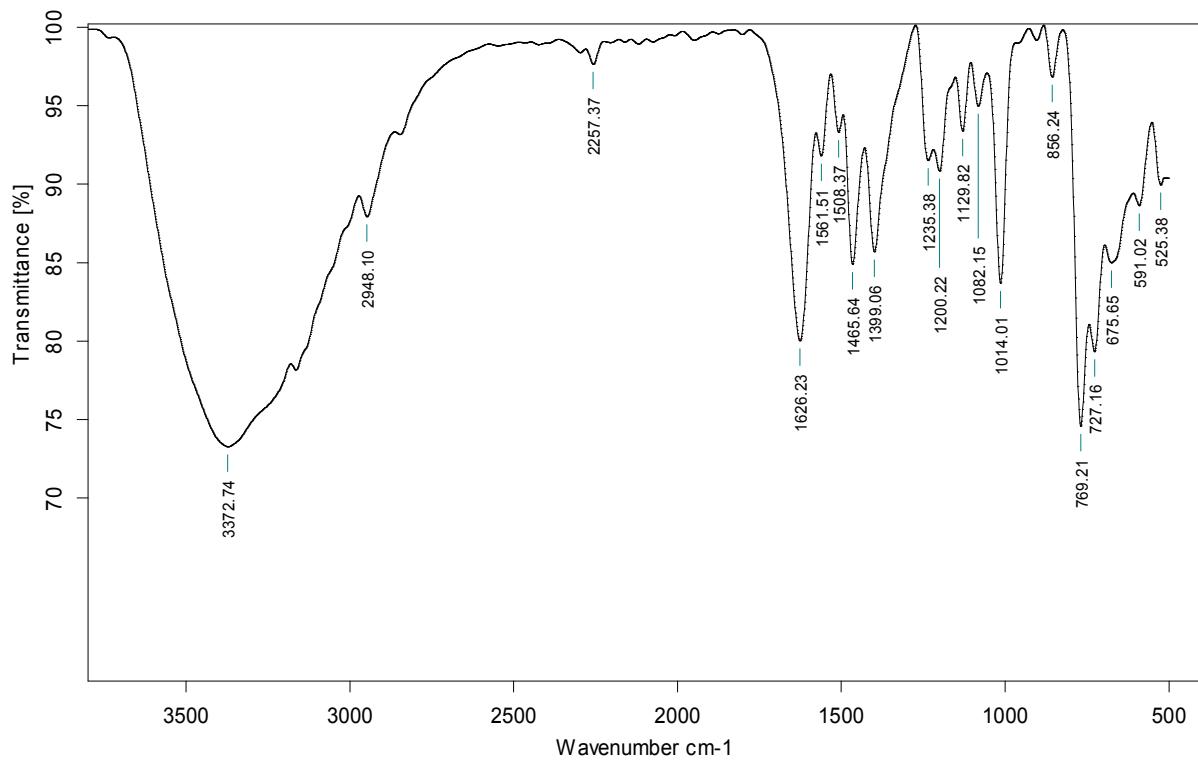


Fig. S12. Neat FT-IR spectrum of complex **2**

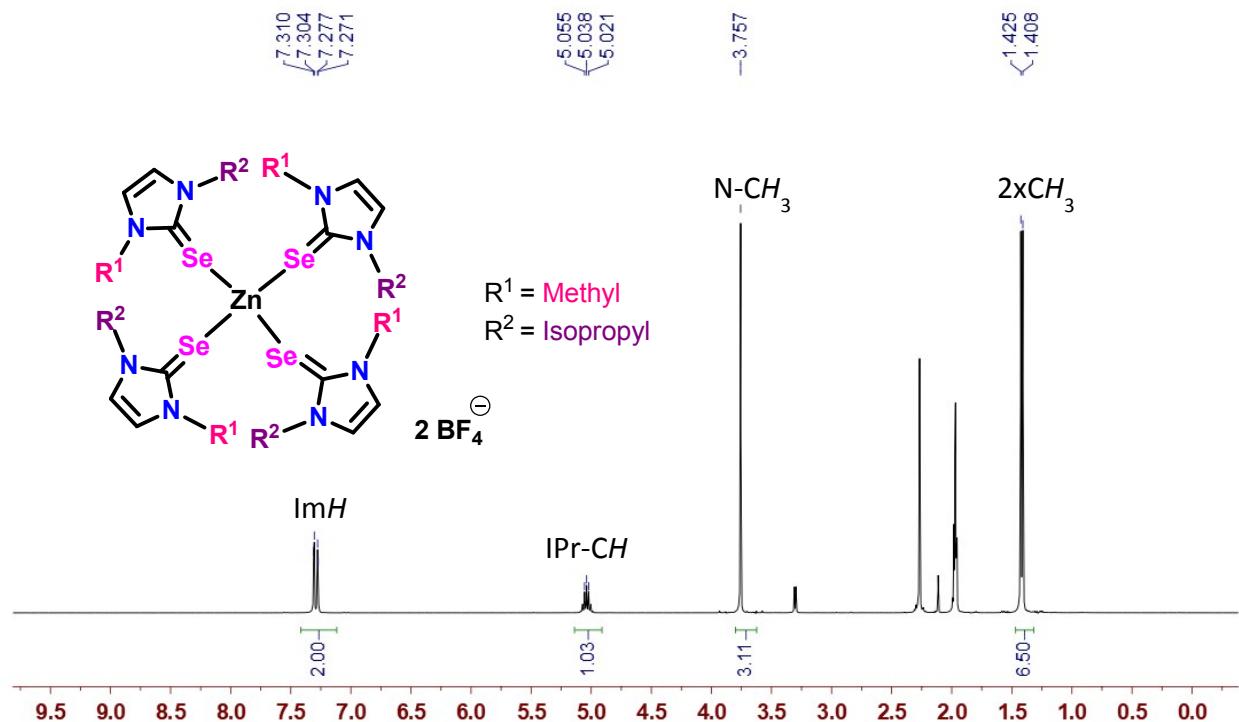


Fig. S13. ^1H NMR spectrum of complex **3** in CD_3CN

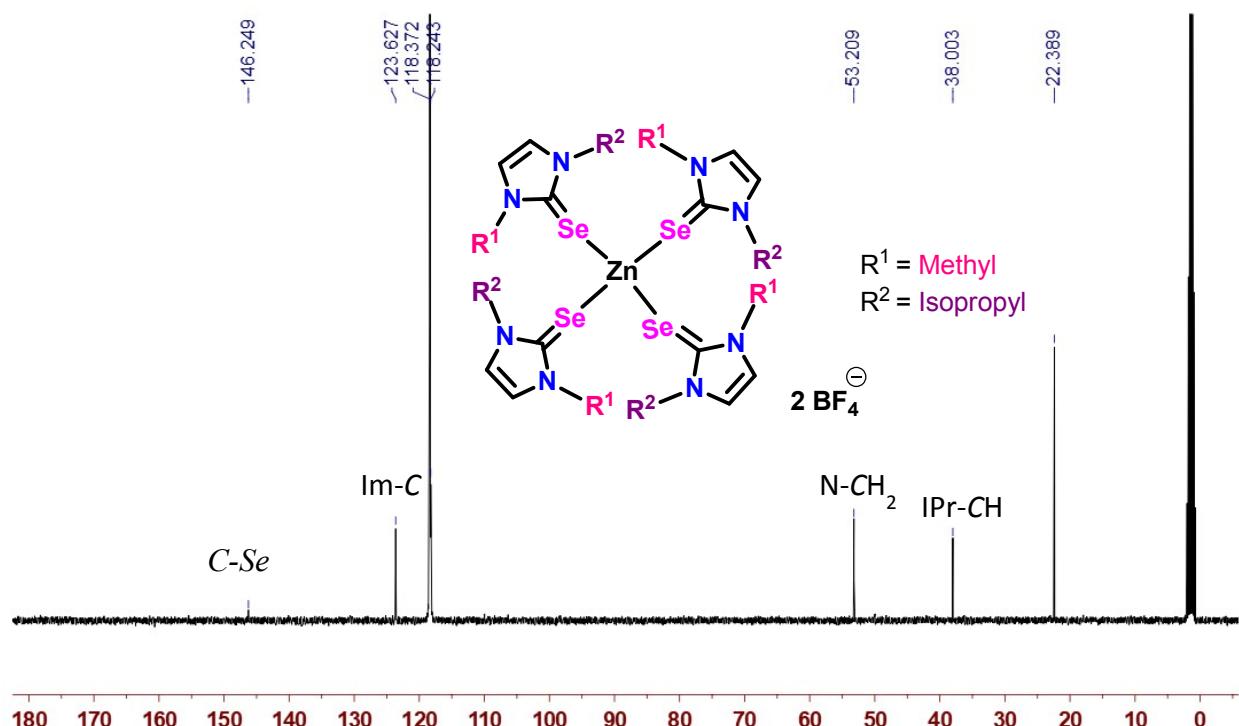


Fig. S14. ^{13}C NMR spectrum of complex **3** in CD_3CN

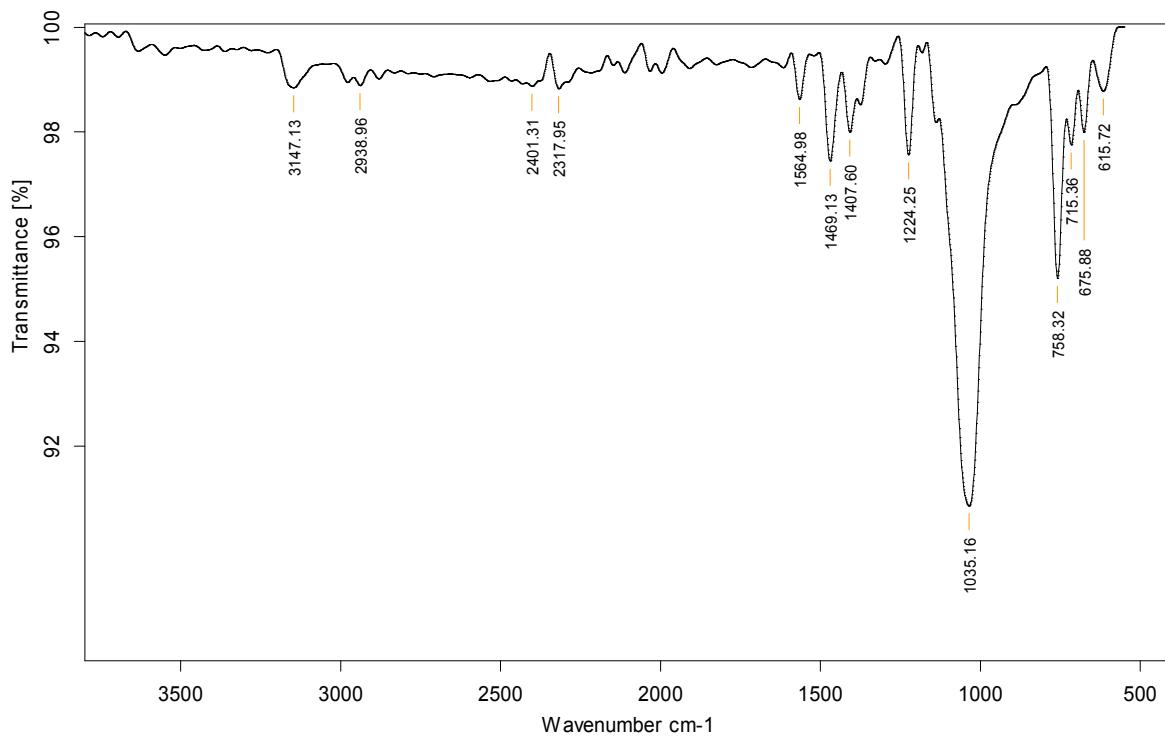


Fig. S15. Neat FT-IR spectrum of complex **3**

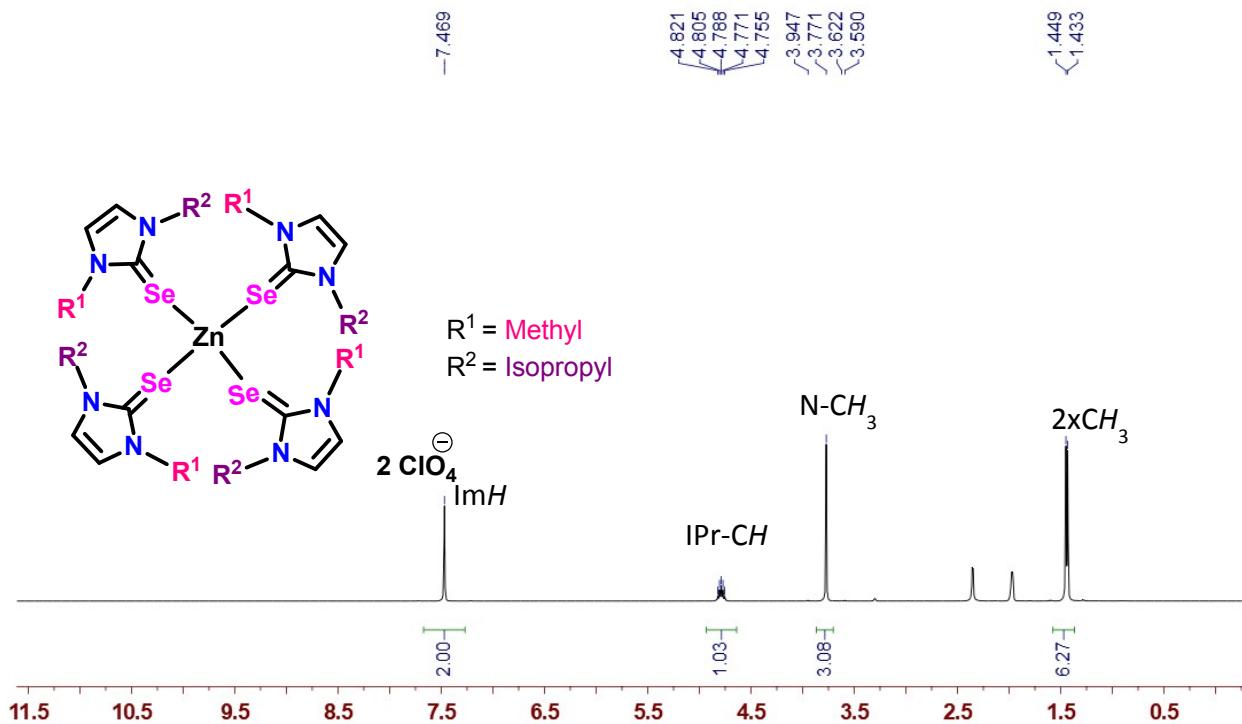


Fig. S16. ^1H NMR spectrum of complex **4** in CD_3CN

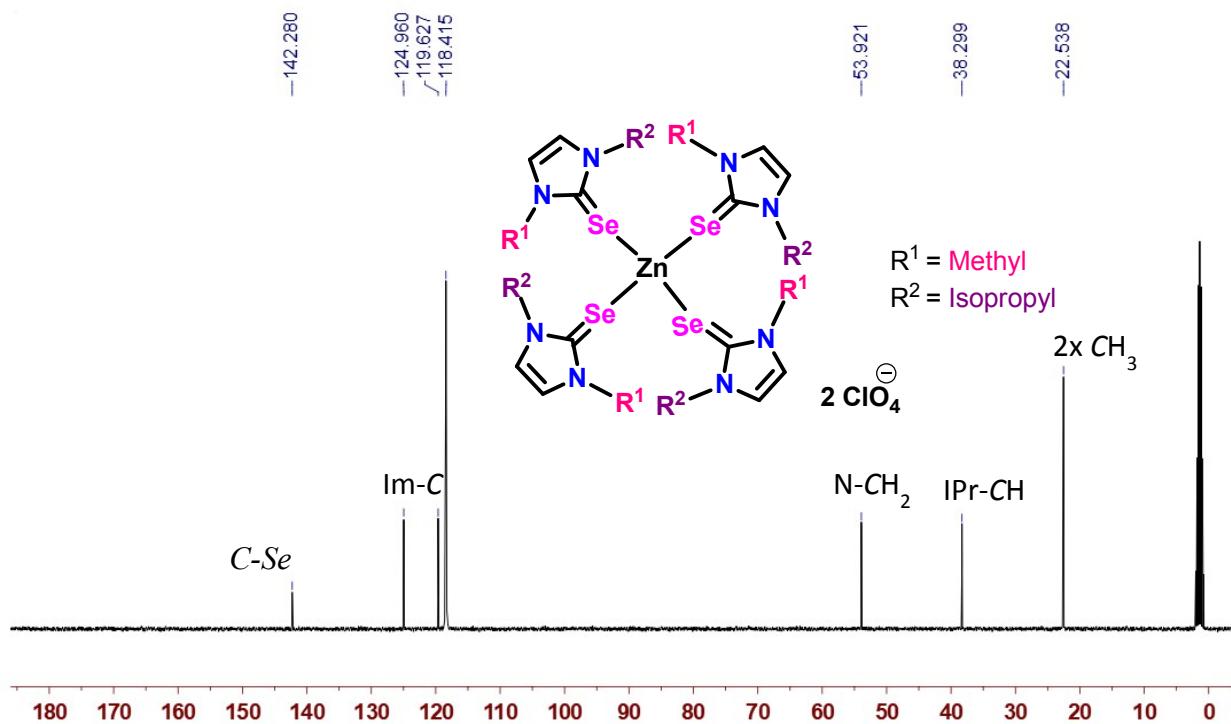


Fig. S17. ^{13}C NMR spectrum of complex 4 in CD_3CN

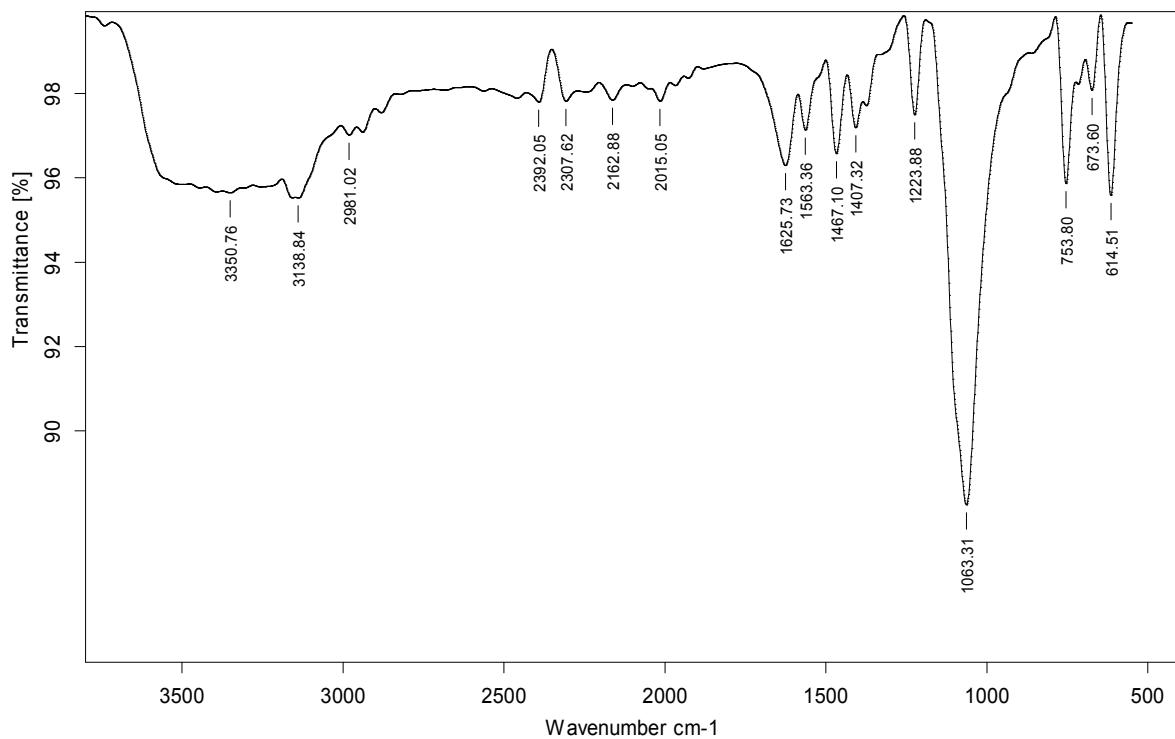


Fig. S18. Neat FT-IR spectrum of complex 4

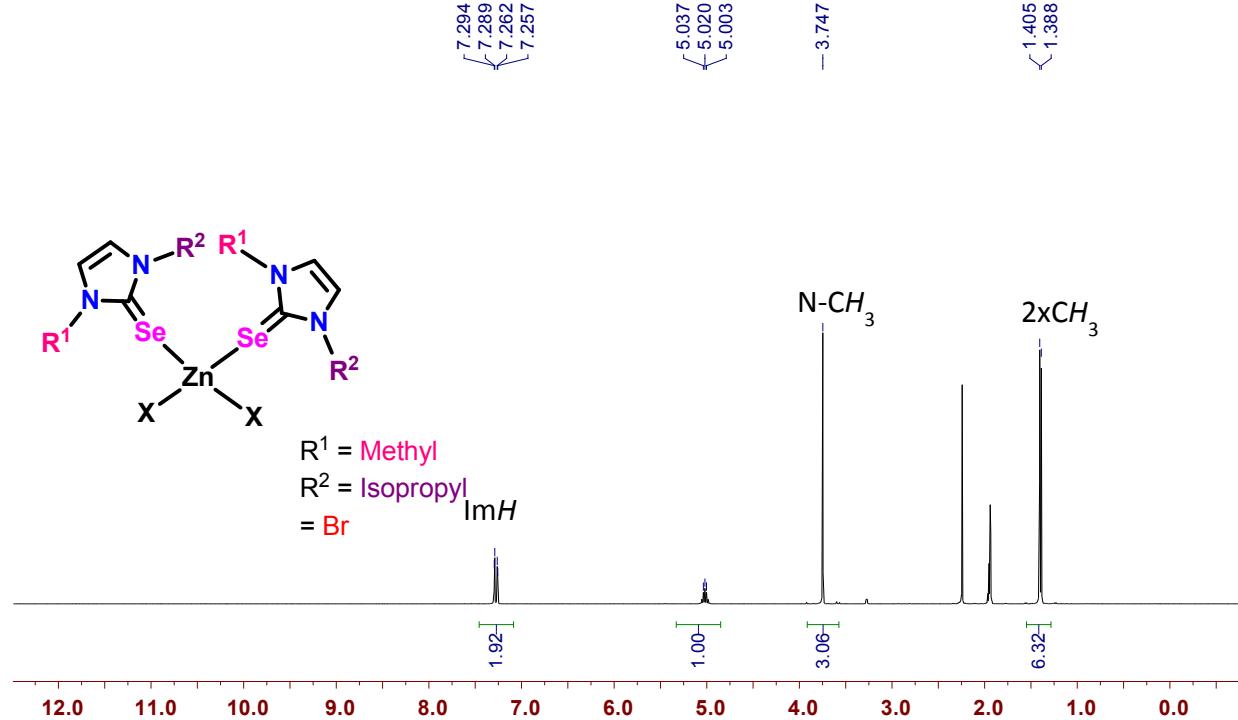


Fig. S19. ^1H NMR spectrum of complex **5** in CD_3CN

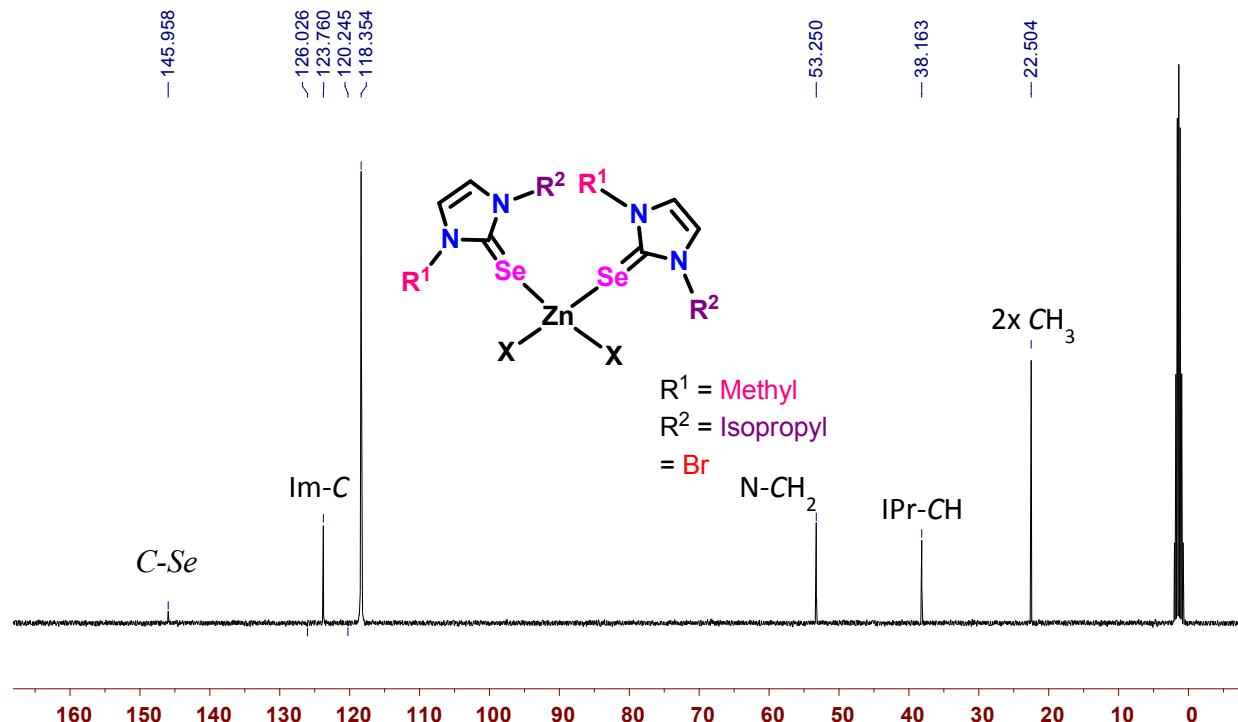


Fig. S20. ^{13}C NMR spectrum of complex **5** in CD_3CN

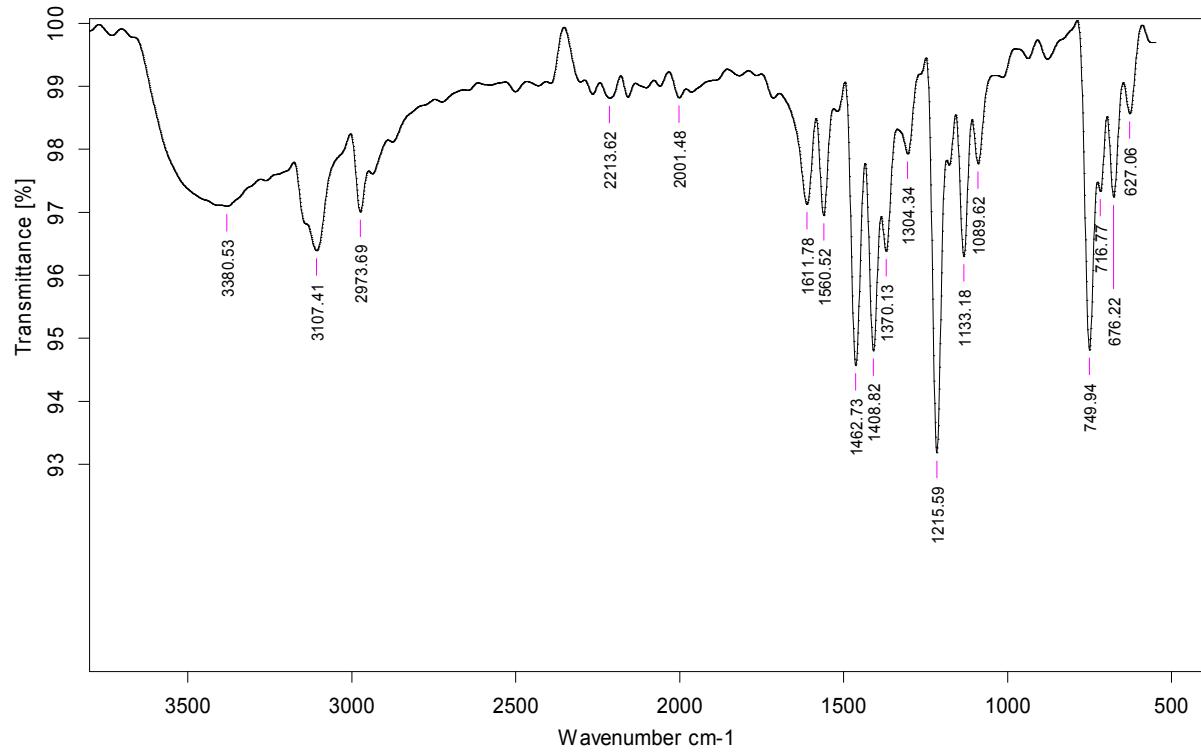
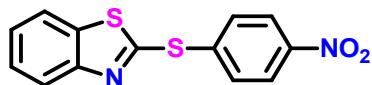


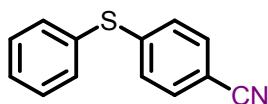
Fig. S21. Neat FT-IR spectrum of complex **5**

1. Compound characterisation data (1a):



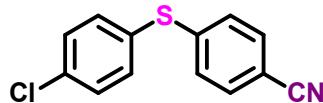
2-((4-nitrophenyl)thio)-1,3-benzothiazole: Chemical Formula: C₁₃H₈N₂O₂S₂; Colourless solid; Yield: 139 mg (80 %); M. P: 85 °C. **¹H NMR (400 MHz, CDCl₃):** δ = 8.07-8.11 (m, 2H), 7.41-7.49(m, 4H), 7.19 (m, 2H). **¹³C NMR (CDCl₃, 100 MHz):** 162.78(ArC), 153.41(ArC), 147.88(ArC), 140.09(ArC), 136.22, 132.68, 131.14, 126.69, 125.57, 124.65, 122.84, 121.20 **FT-IR (neat, ̄):** 1570(s), 1502(s), 1388(m), 1329(s), 1080(s), 1009(m), 844(m), 814(m), 738(s), 504(w).

2. Compound characterisation data (2a):



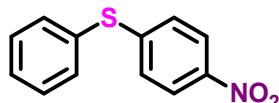
4-(phenylthio)benzonitrile : Chemical Formula: C₁₃H₉NS; Colourless solid; Yield: 116 mg (75 %); M. P: 80 °C. **¹H NMR (400 MHz, CDCl₃):** δ = 7.42-7.52 (m, 7H), 7.13 (m, 2H), **¹³C NMR (CDCl₃, 100 MHz):** 145.77, 134.55, 132.40, 130.81, 129.44, 127.30, 118.85, 108.67. **FT-IR (neat, ̄):** 2217, 1581(s), 1470(s), 1389(m), 1180(m), 1078(s), 1006(m), 814(s), 740(m), 583(m), 537(m), 496(s).

3. Compound characterisation data (3a):



4-((4-chlorophenyl)thio)benzonitrile: Chemical Formula: C₁₃H₈NSCl; Colourless solid; Yield: 123 mg (74 %); M. P: 88 °C. **¹H NMR (400 MHz, CDCl₃):** δ = 7.49-7.51 (m, 2H), 7.38-7.45 (m, 4H), 7.18 (m, 2H). **¹³C NMR (CDCl₃, 100 MHz):** 144.92, 139.57, 135.75, 133.40, 132.52, 130.17, 129.71, 129.56, 127.57, 116.65, 110.79, 109.16. **FT-IR (neat, ̄):** 2217, 1582(s), 1471(s), 1389(m), 1327(s), 1079(s), 1008(m), 815(s), 737(s), 539(m), 485(s).

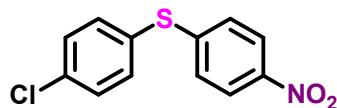
4. Compound characterisation data (4a):



(4-nitrophenyl)(phenyl) sulfane : Chemical Formula: C₁₂H₉NO₂S; yellow Colour solid; Yield: 104 mg (90 %); M. P: 86 °C. **¹H NMR (400 MHz, CDCl₃):** δ = 8.04-8.08 (m, 2H), 7.44-7.56 (m, 5H), 7.18 (m, 2H). **¹³C NMR (CDCl₃, 100 MHz):** 148.52, 145.37, 134.76, 130.47, 130.05,

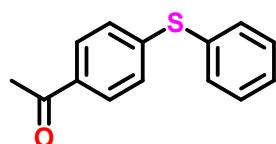
129.69, 126.68, 124.05. **FT-IR (neat, $\bar{\nu}$):** 1577(s), 1507(s), 1327(s), 1177(m), 1076(s), 1012(m), 840(s), 739(s), 685(s), 507(s).

5. Compound characterisation data (5a):



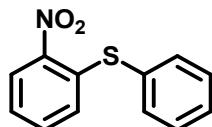
(4-chlorophenyl)(4-nitrophenyl)sulfane: Chemical Formula: C₁₂H₈NO₂SCl; Colourless solid; Yield: 113 mg (85 %); **M. P:** 90 °C. **¹H NMR (400 MHz, CDCl₃):** δ = 8.23 (dd, J=8.3, 1.4 Hz, 1H), 7.22-7.53 (m, 6H), 6.86 (dd, J=8.2, 1.2 Hz, 1H). **¹³C NMR (CDCl₃, 100 MHz):** 145.12, 137.11, 136.74, 136.53, 135.57, 133.40, 129.63, 128.25, 126.84, 125.28. **FT-IR (neat, $\bar{\nu}$):** 1576(s), 1501(s), 1388(m), 1327(s), 1079(s), 1007(m), 834(m), 812(m), 737(s), 677(w), 533(w).

6. Compound characterisation data(6a):



1-(4-Phenylsulfonylphenyl)ethanone: Chemical Formula: C₁₄H₁₂OS; Colourless solid; Yield: 85 mg (73 %); **M. P:** 69 °C. **¹H NMR (400 MHz, CDCl₃):** δ = 7.82(m, 2H), 7.49 (dd, J=6.6, 4.1 Hz, 2H), 7.40 (m, 3H), 7.20 (m, 2H), 2.55 (s, 3H). **¹³C NMR (100MHz, CDCl₃):** δ 197.20, 144.97, 134.47, 133.91, 132.06, 129.71, 128.92, 128.92, 127.45, 26.51. **FT-IR (neat, $\bar{\nu}$):** 3337(w), 1678(s), 1585(s), 1474(w), 1398(w), 1358(m), 1264(s), 1090(m), 1016(s), 957(m), 821(m), 748(m), 692(m), 587(w).

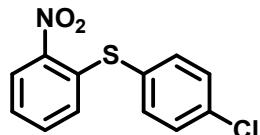
7. Compound characterisation data (7a):



(3-nitrophenyl)(phenyl)sulfane: Chemical Formula: C₁₂H₉O₂NS; yellow Colour solid; Yield: 100 mg (80 %); **M. P:** 82 °C. **¹H NMR (400 MHz, CDCl₃):** δ = 8.22 (dd, J=8.2, 1.4 Hz, 1H), 7.59 (m, 2H), 7.47(m, 3H), 7.21 (m, 2H), 6.85(dd, J=8.2, 1.2 Hz, 1H) **¹³C NMR (CDCl₃, 100 MHz):** 145.01, 139.47, 135.91, 133.43, 131.17, 130.93, 130.09, 129.01, 128.33, 126.45, 125.75,

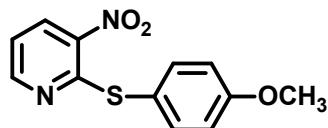
124.98. **FT-IR (neat, $\bar{\nu}$):** 1583(s), 1510(s), 1447(m), 1333(s), 1299(m), 1165(w), 1104(s), 1043(s), 906(s), 851(m), 724(s), 485(s).

8. Compound characterisation data (8a):



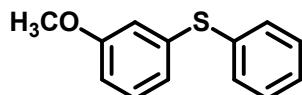
(4-chlorophenyl)(3-nitrophenyl)sulfane: Chemical Formula: $C_{12}H_8NO_2SCl$; yellow colour solid; Yield: 120 mg (78 %); **M. P:** 93 °C. **1H NMR (400 MHz, $CDCl_3$):** $\delta = 8.23$ (dd, $J=8.3, 1.4$ Hz, 1H), 7.43-7.55 (m, 4H), 7.37 (m, 2H), 6.85(dd, $J=8.2, 1.2$ Hz 1H). **^{13}C NMR ($CDCl_3$, 100 MHz):** 145.12, 138.74, 137.11, 136.53, 133.57, 130.41, 129.61, 128.23, 125.86, 125.27. **FT-IR (neat, $\bar{\nu}$):** 1570(s), 1499(s), 1330(m), 1295(s), 1085(s), 815(m), 727(s), 490(m).

9. Compound characterisation data (9a):



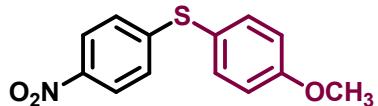
2-(4-methoxyphenyl)-3-nitropyridine : Chemical Formula: $C_{12}H_{10}N_2O_3S$; yellow Colour solid; Yield: 64 mg (58 %); **M. P:** 138 °C. **1H NMR (400 MHz, $CDCl_3$):** $\delta = 7.84$ (m, 2H), 7.55 (m, 3H), 7.04(d, 2H), 4.19(s, 3H) **^{13}C NMR ($CDCl_3$, 100 MHz):** 158.57, 140.62, 137.25, 135.54, 131.87, 129.84, 129.79, 129.28, 128.93, 126.07, 118.00, 38.73. **FT-IR (neat, $\bar{\nu}$):** 2920(s), 2854(m), 1706(s), 1580(m), 1458(s), 1338(s), 1286(s), 1175(s), 1120(m), 1071(m), 1025(m), 966(m), 852(s), 740(m), 696(s), 614(m), 547(m), 511(m).

10. Compound characterisation data (10a):



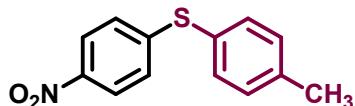
(3-methoxyphenyl)(phenyl)sulfane: Chemical Formula: $C_{13}H_{12}OS$; Colourless liquid; Yield: 58 mg (60 %). **1H NMR (400 MHz, $CDCl_3$):** $\delta = 7.36$ (m, 2H), 7.31 (m, 2H), 7.18-7.26 (m, 2H), 6.73-6.91(m, 3H), 3.75(s, 3H) **^{13}C NMR ($CDCl_3$, 100 MHz):** 160.06, 137.25, 135.26, 131.45, 129.98, 129.25, 127.28, 122.96, 115.90, 112.80, 55.39. **FT-IR (neat, $\bar{\nu}$):** 2922(m), 1580(s), 1470(s), 1283(m), 1236(s), 1179(m), 1035(s), 966(m), 852(s), 740(s), 685(s), 560(m), 502(s).

11. Compound characterisation data (11a):



(4-methoxyphenyl) (4-nitrophenyl) sulfane: Chemical Formula: C₁₃H₁₁NO₃S; yellow colour solid; Yield: 92 mg (72 %); M. P: 82-85 °C. **¹H NMR (400 MHz, CDCl₃):** δ = 8.02-8.05 (m, 2H), 7.45-7.53 (m, 2H), 7.01-7.13 (m, 4H), 3.82 (s, 3H). **¹³C NMR (CDCl₃, 100 MHz):** 159.72, 147.98, 145.17, 136.87, 132.01, 126.15, 123.86, 121.68, 117.64, 111.80, 55.98. **FT-IR (neat, $\bar{\nu}$):** 2892(s), 2822(m), 1561(s), 1493(s), 1452(s), 1317(s), 1259(s), 1230(m), 1061(s), 1005(s), 833(s).

12. Compound characterisation data (12a):



(4-nitrophenyl) (p-tolyl) sulfane: Chemical Formula: C₁₃H₁₁NO₂S; yellow colour ; Yield: 95 mg (78 %). M. P: 85-90 °C. **¹H NMR (400 MHz, CDCl₃):** δ = 7.96 (d, J= 9.1 Hz, 2H), 7.35 (m, 2H), 7.19 (m, 2H), 7.05 (m, 2H), 2.34 (s, 3H). **¹³C NMR (CDCl₃, 100 MHz):** 148.60, 143.81, 138.45, 134.05, 131.59, 129.63, 128.85, 125.45, 123.97, 122.94, 20.30. **FT-IR (neat, $\bar{\nu}$):** 2894(m), 2818(m), 2231(w), 1563(s), 1495(s), 1456(w), 1321(s), 1263(m), 1072(m), 1009(m), 895(s), 836(m).

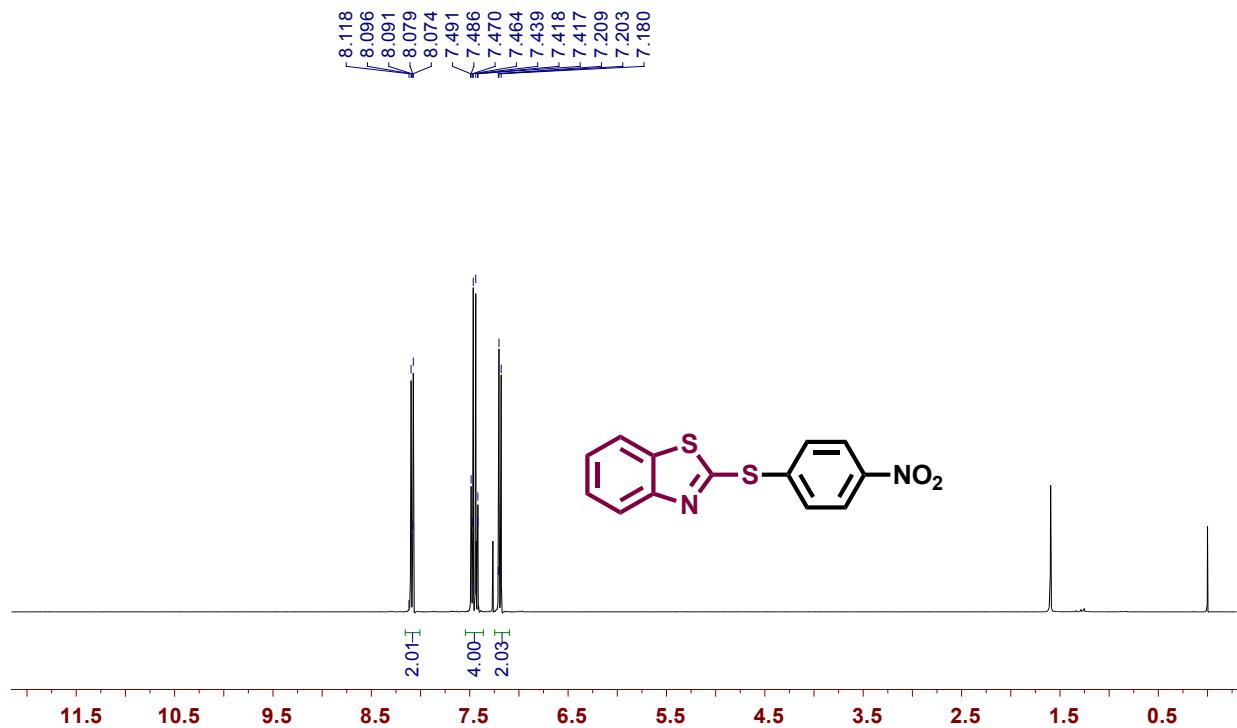


Fig. S22. ¹H NMR spectrum of compound **1a** in CDCl_3

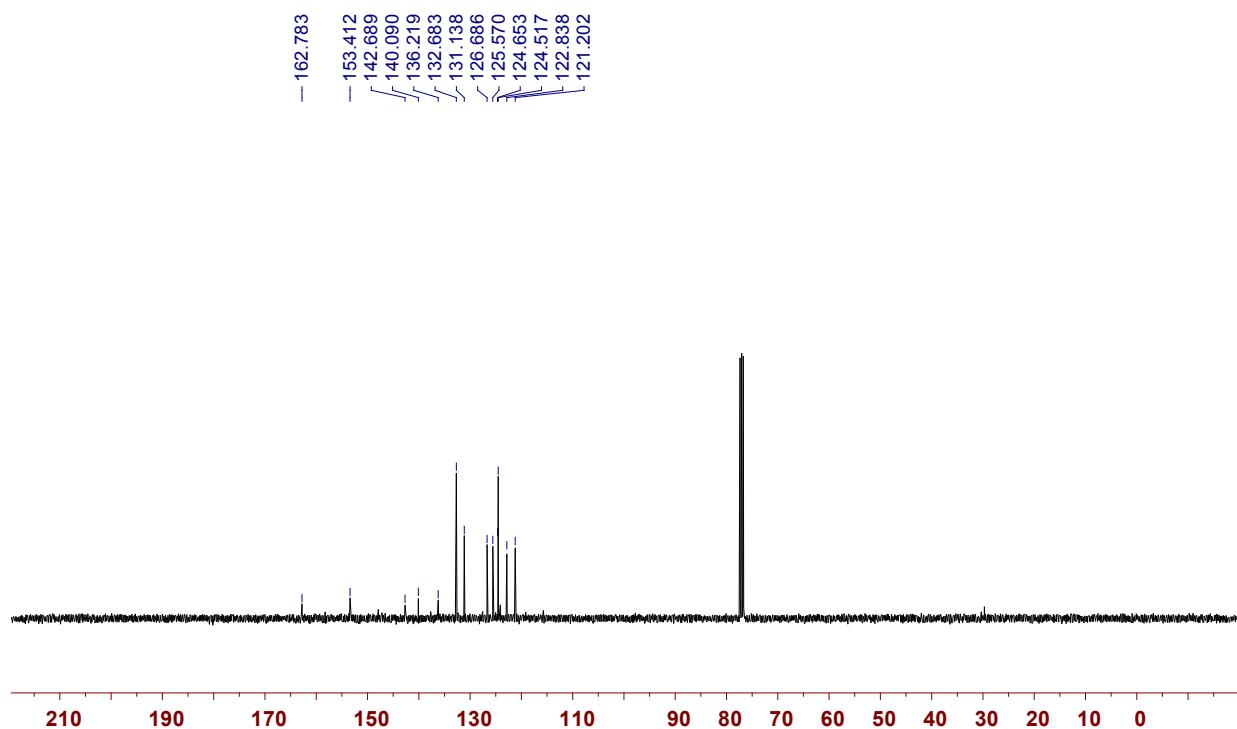


Fig. S23. ¹³C NMR spectrum of compound **1a** in CDCl_3

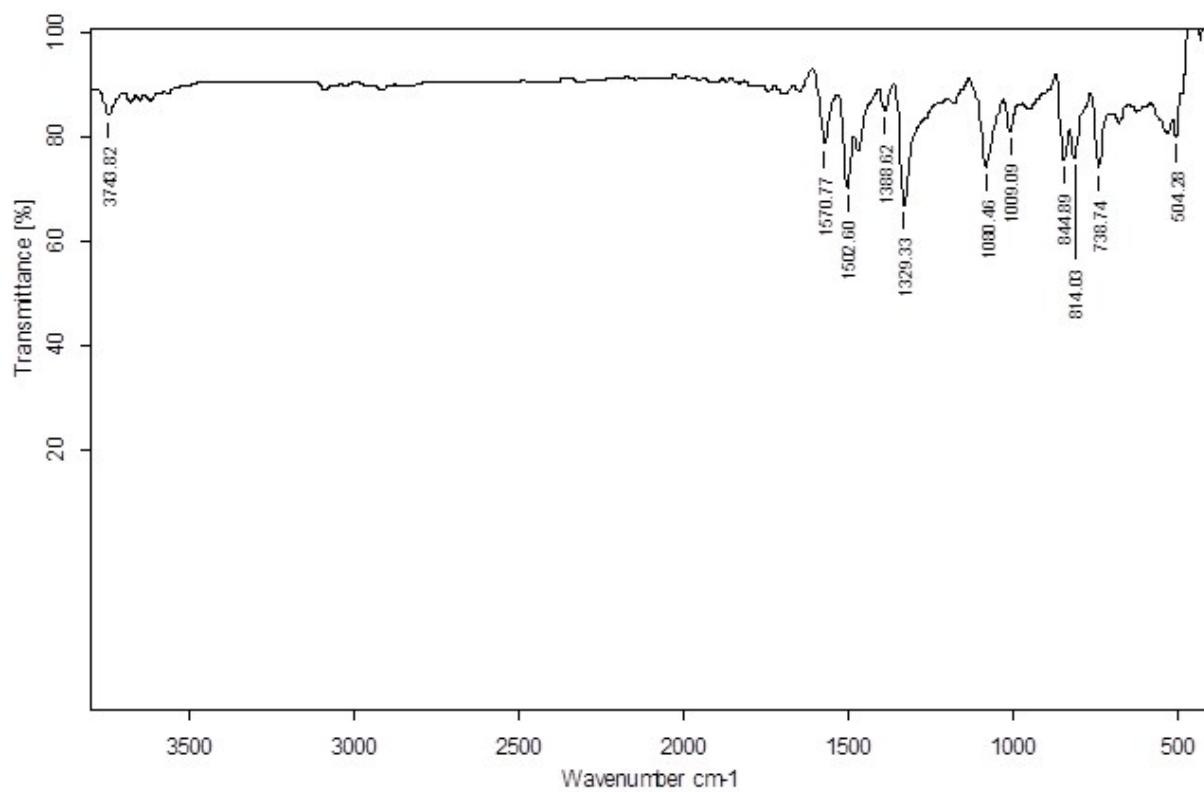


Fig. S24. Neat FT-IR spectrum of complex **1a**

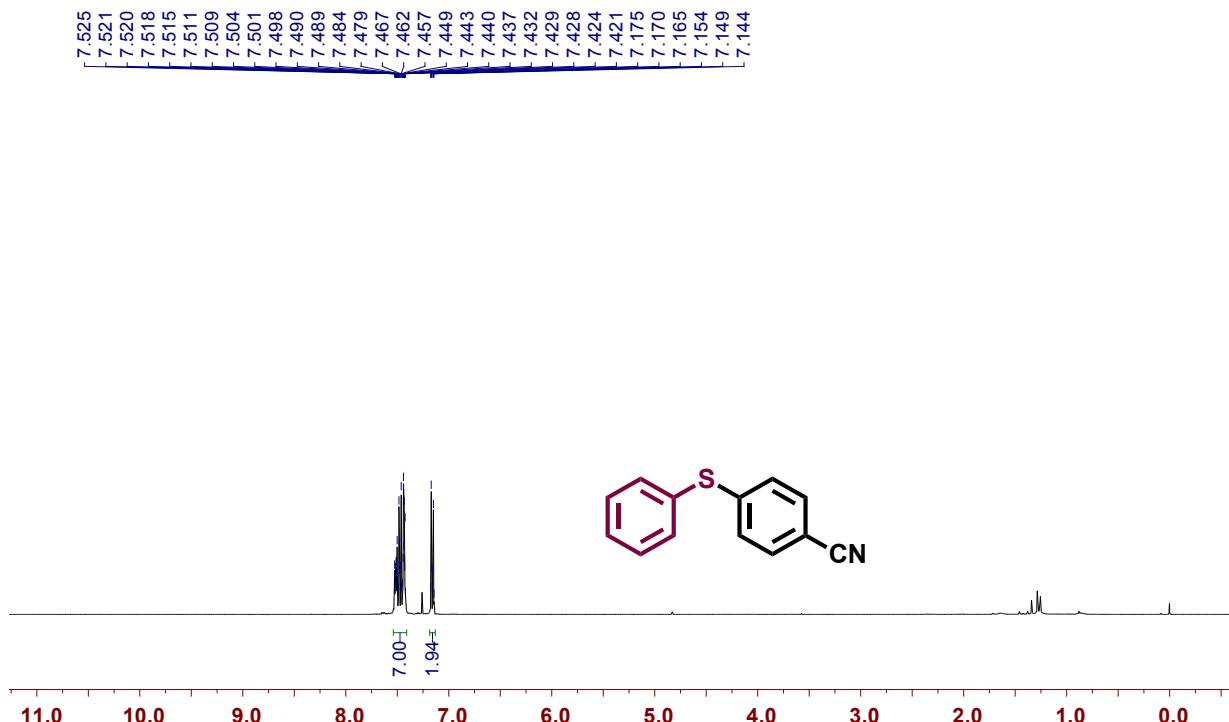


Fig. S25. ^1H NMR spectrum of compound **2a** in CDCl_3

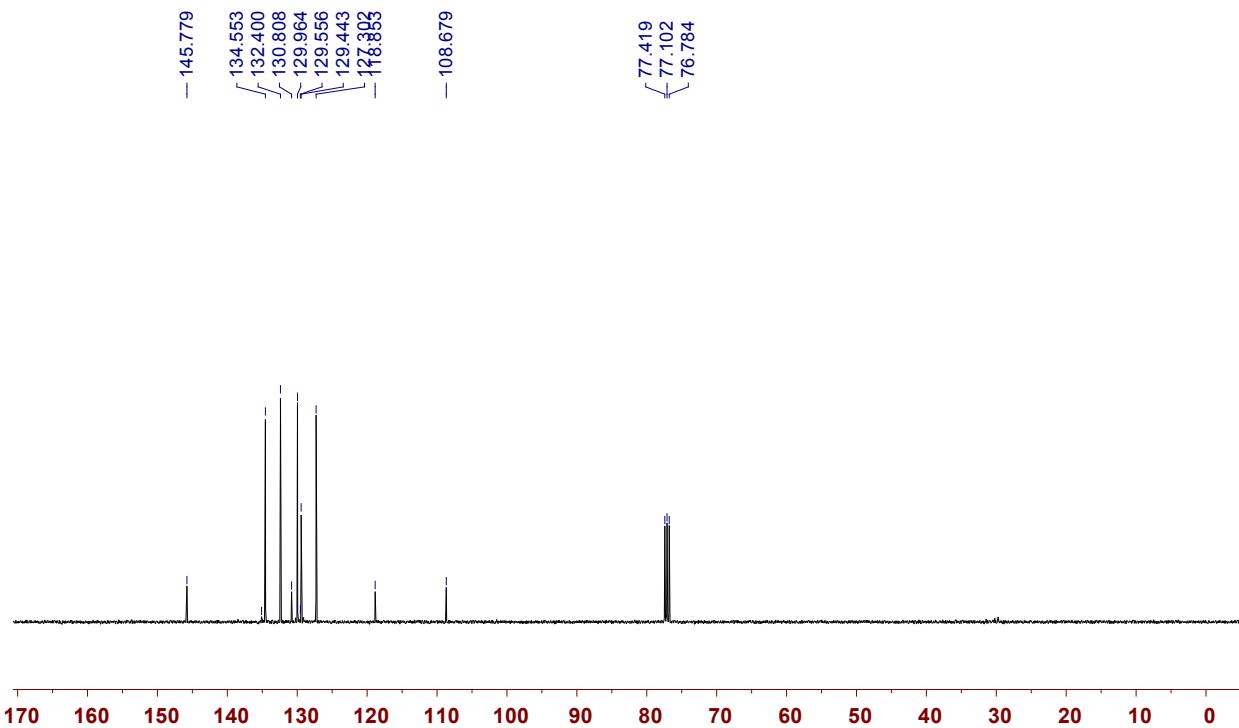


Fig. S26. ^{13}C NMR spectrum of compound **2a** in CDCl_3

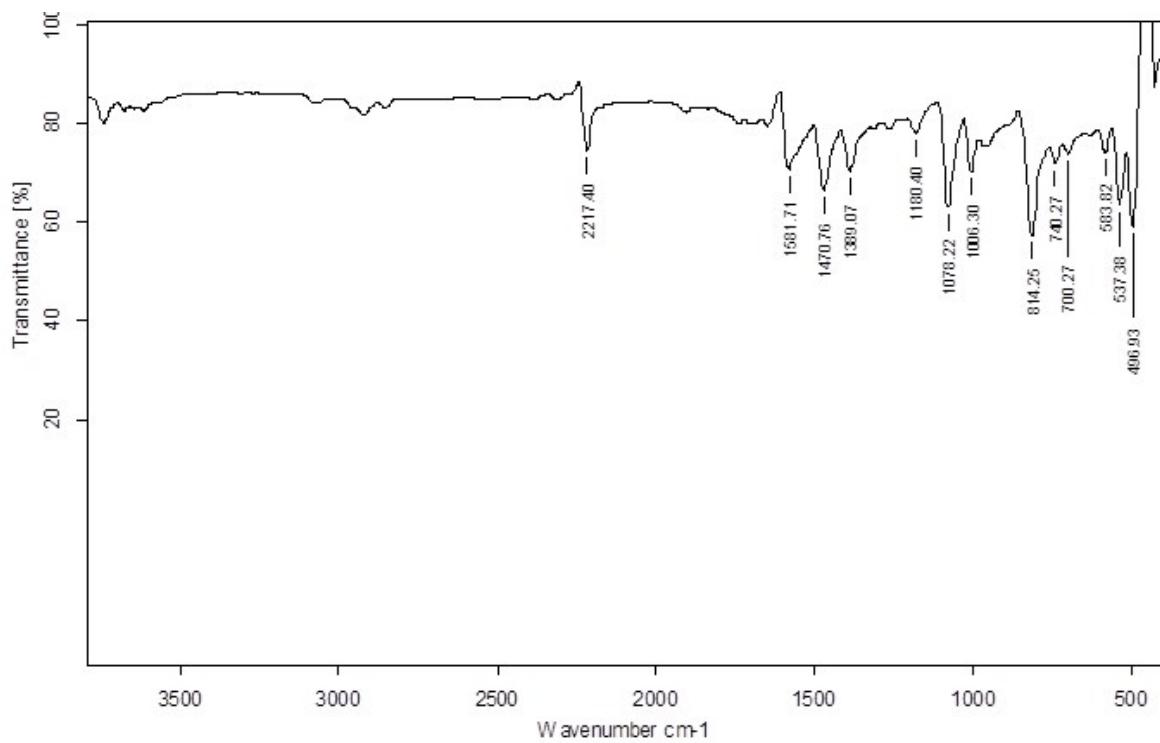


Fig. S27. Neat FT-IR spectrum of complex **2a**

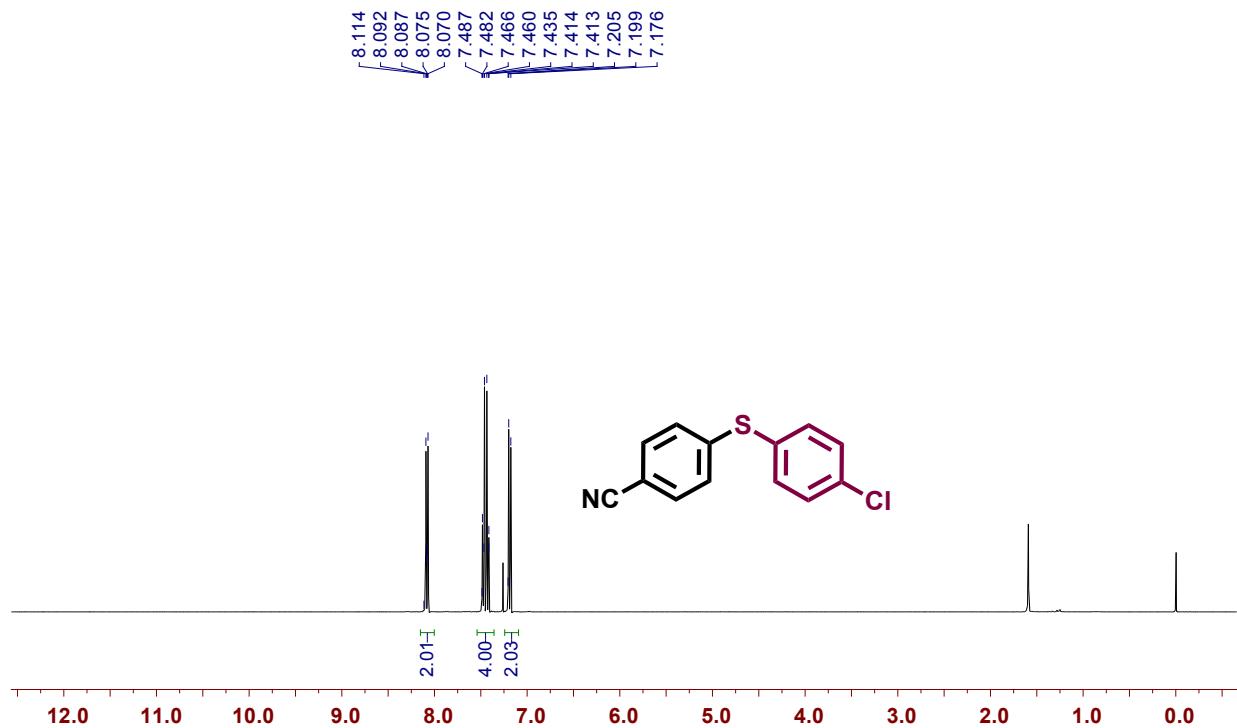


Fig. S28. ¹H NMR spectrum of compound 3a in CDCl₃

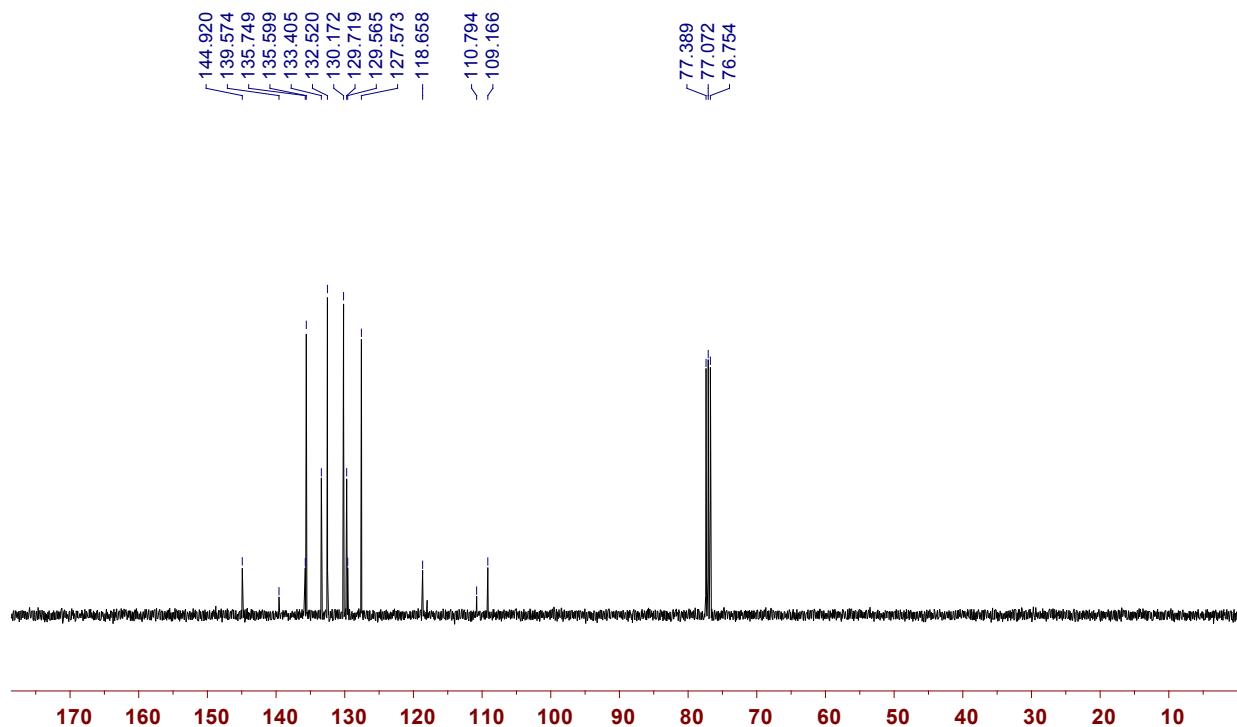


Fig. S29. ¹³C NMR spectrum of compound 3a in CDCl₃

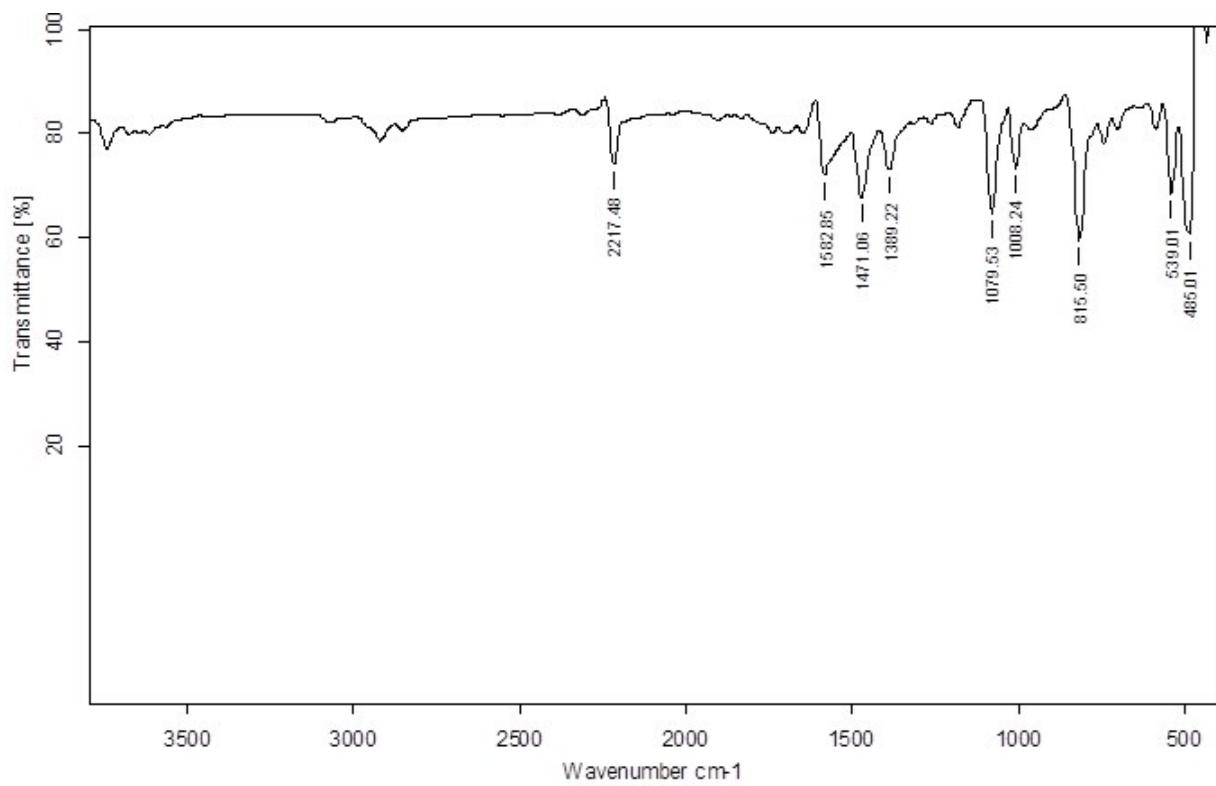


Fig. S30. Neat FT-IR spectrum of complex **3a**

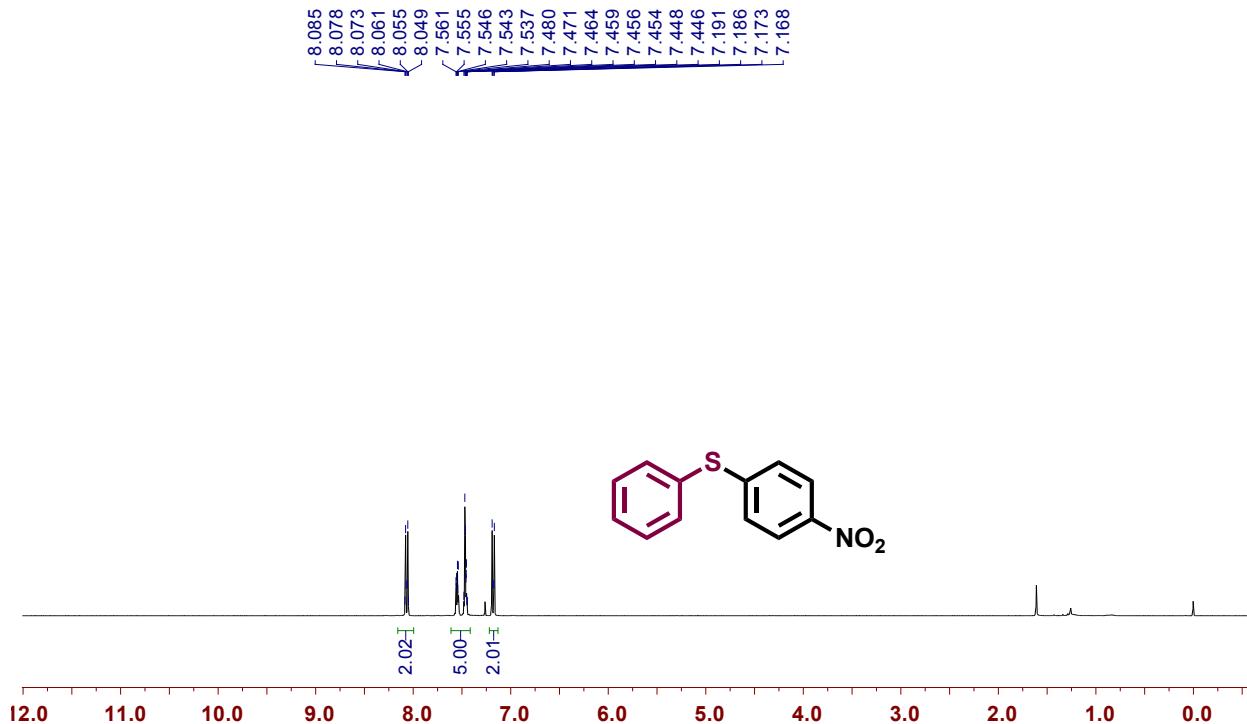


Fig. S31. ^1H NMR spectrum of compound **4a** in CDCl_3

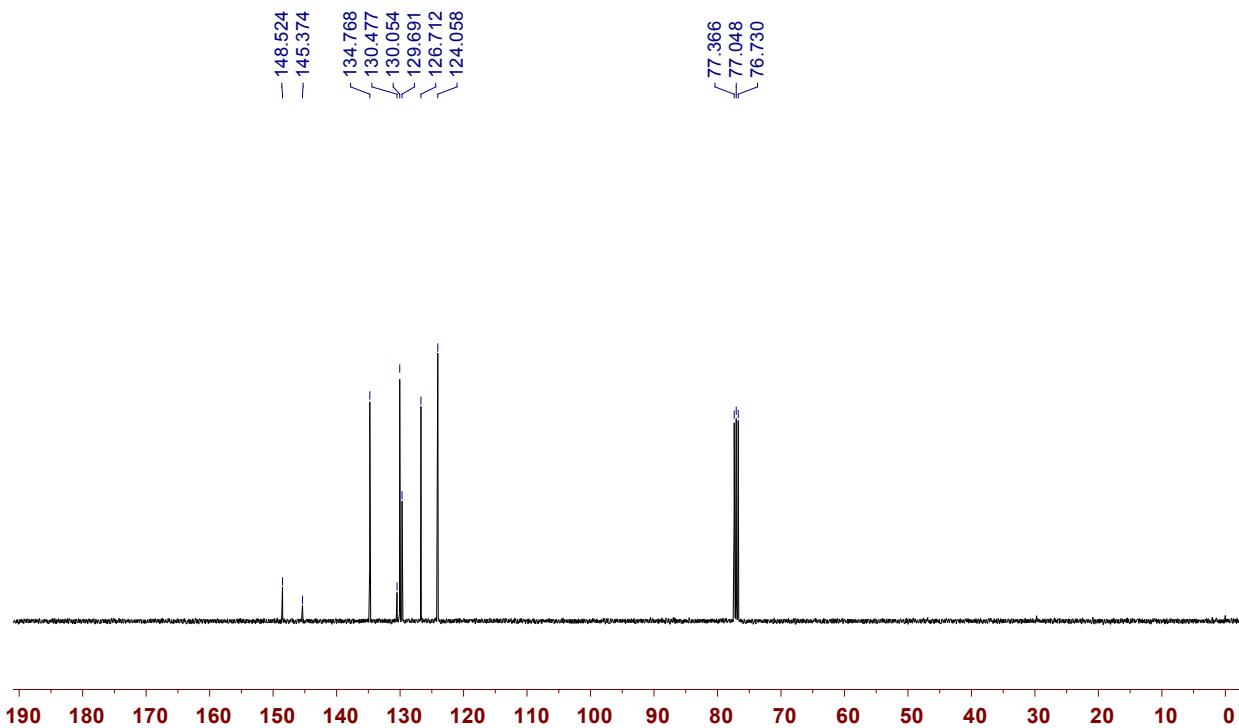


Fig. S32. ^{13}C NMR spectrum of compound **4a** in CDCl_3

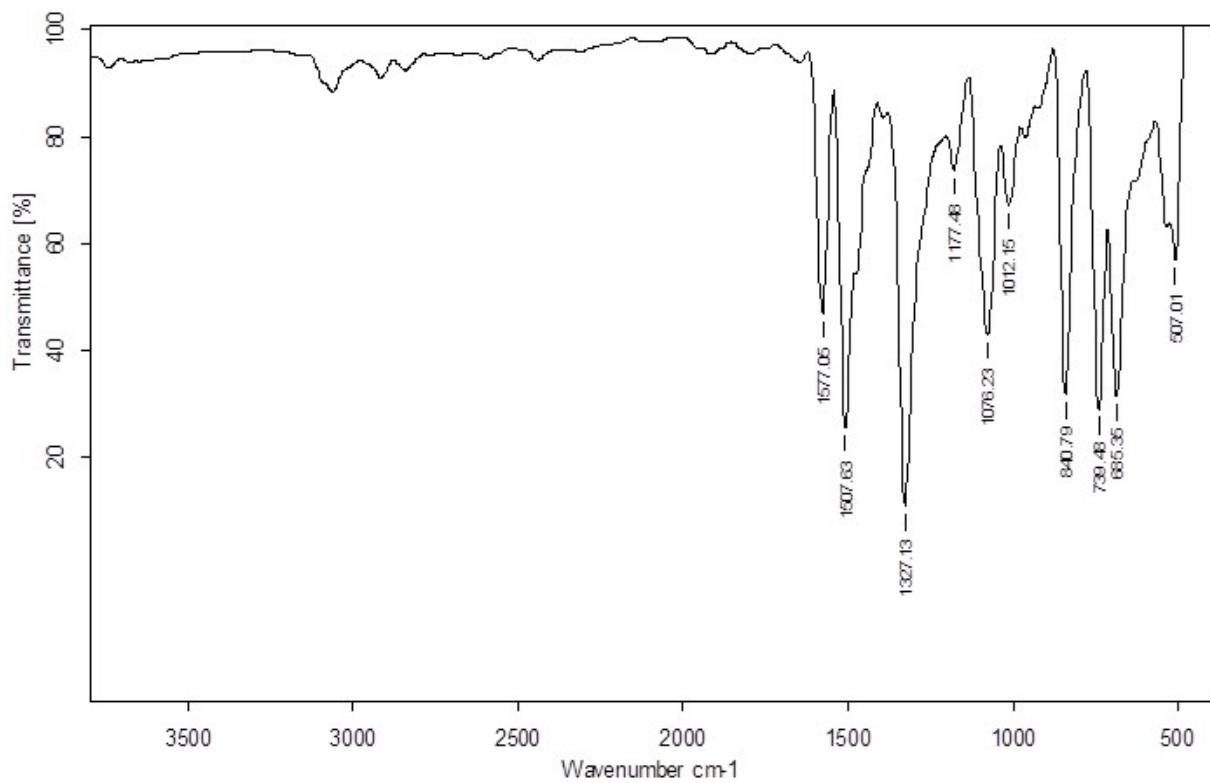


Fig. S33. Neat FT-IR spectrum of complex **4a**

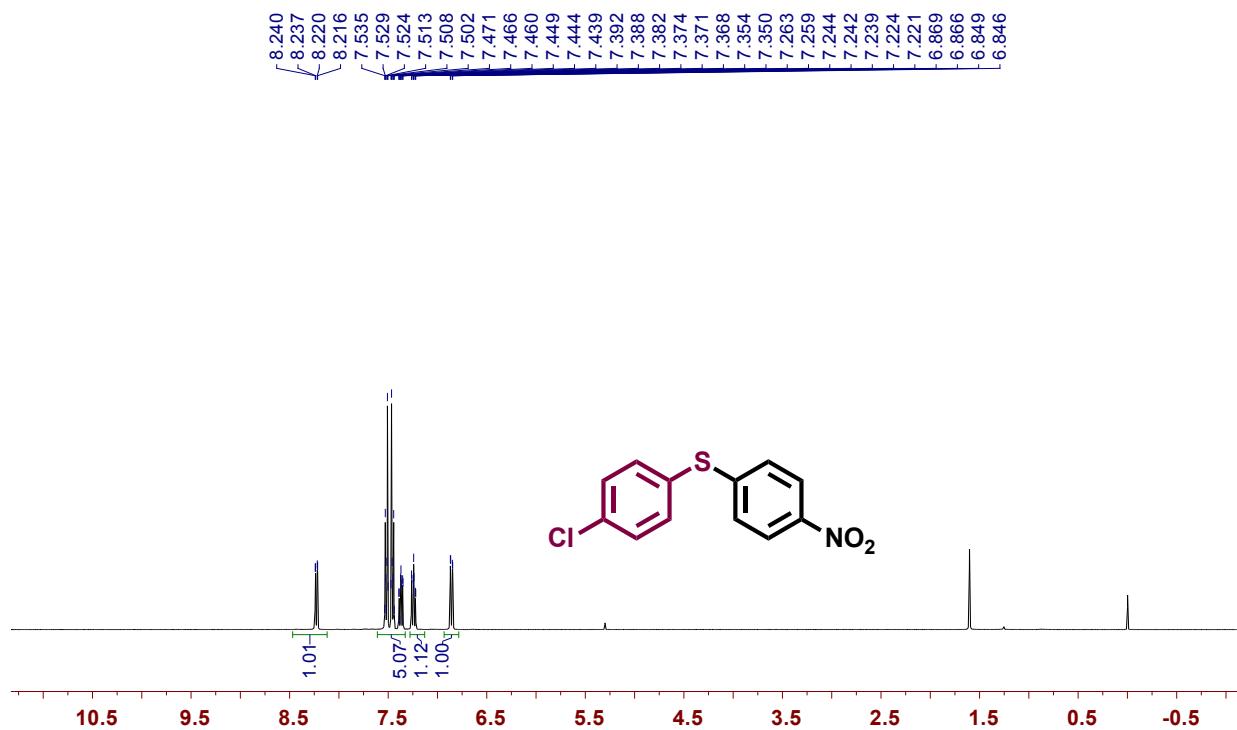


Fig. S34. ^1H NMR spectrum of compound **5a** in CDCl_3

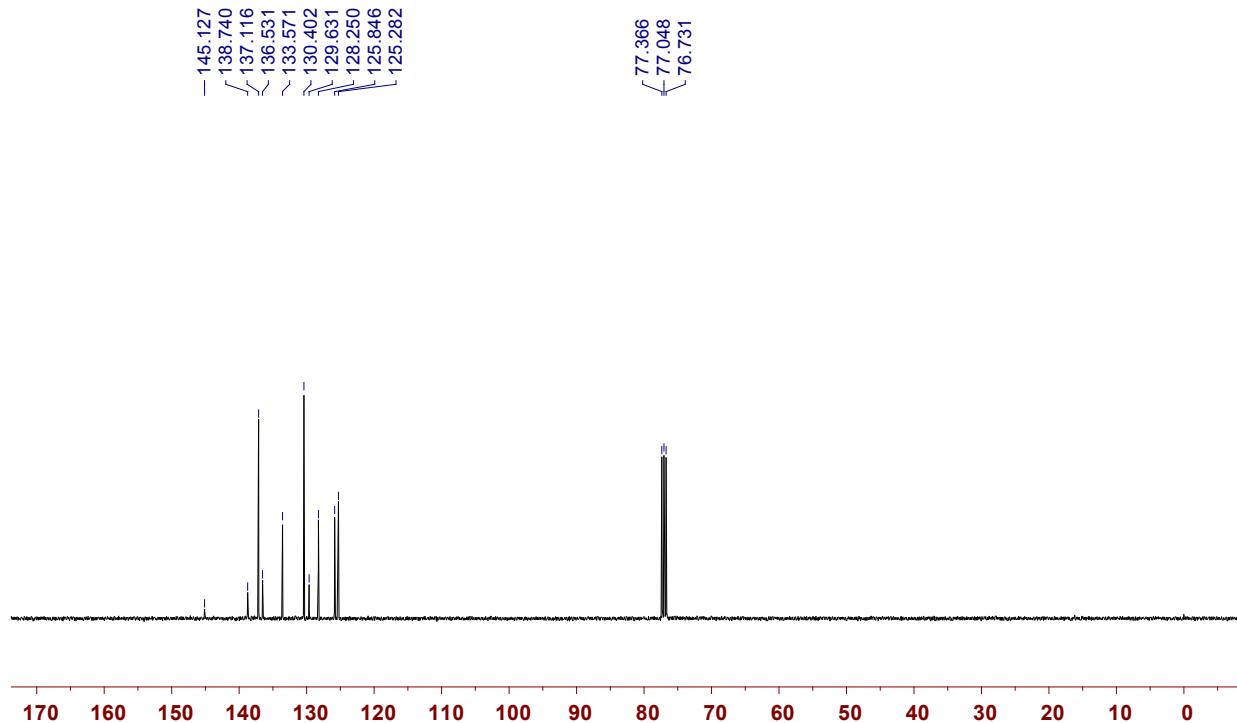


Fig. S35. ^{13}C NMR spectrum of compound **5a** in CDCl_3

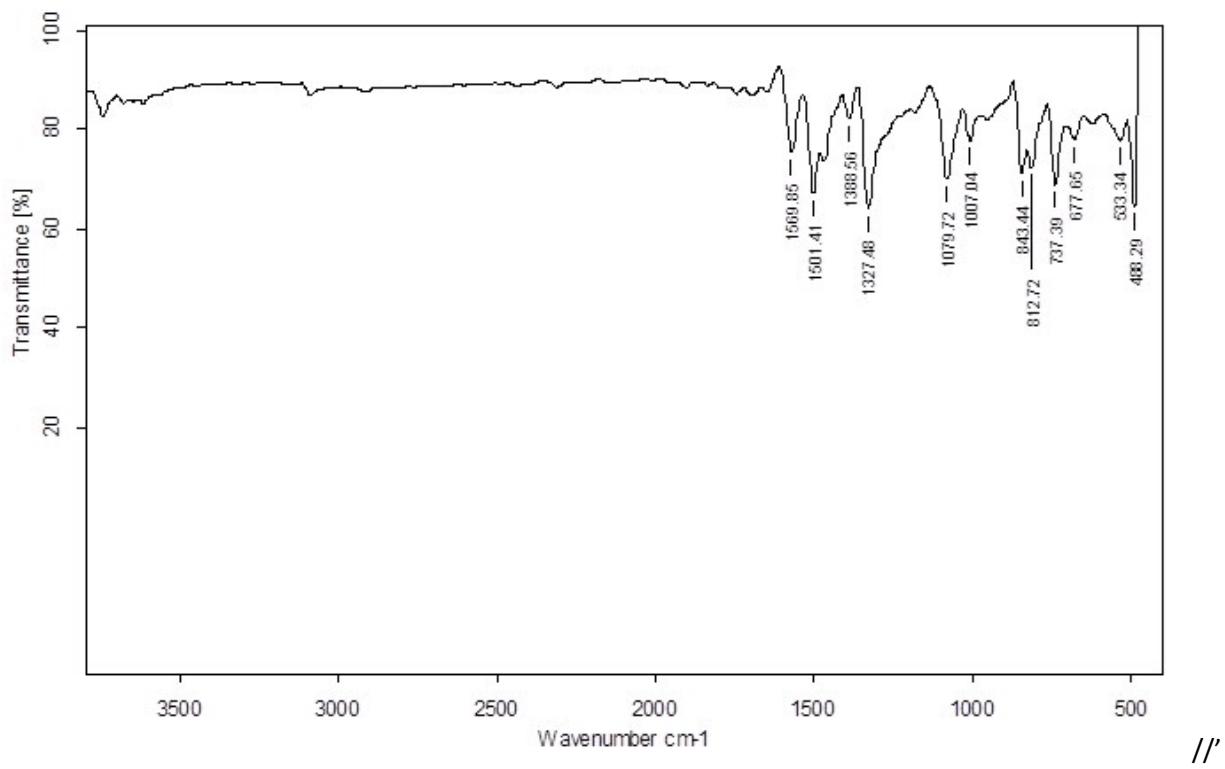


Fig. S36. Neat FT-IR spectrum of complex **5a**

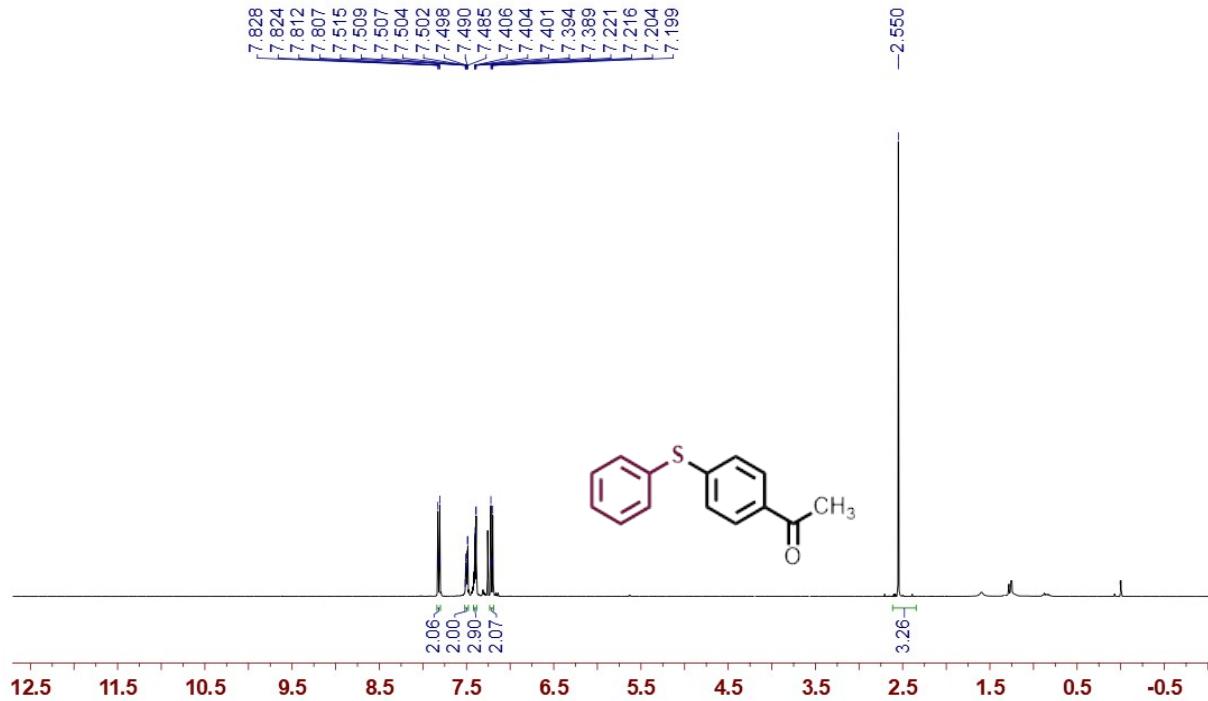


Fig. S37. ¹H NMR spectrum of compound **6a** in CDCl₃

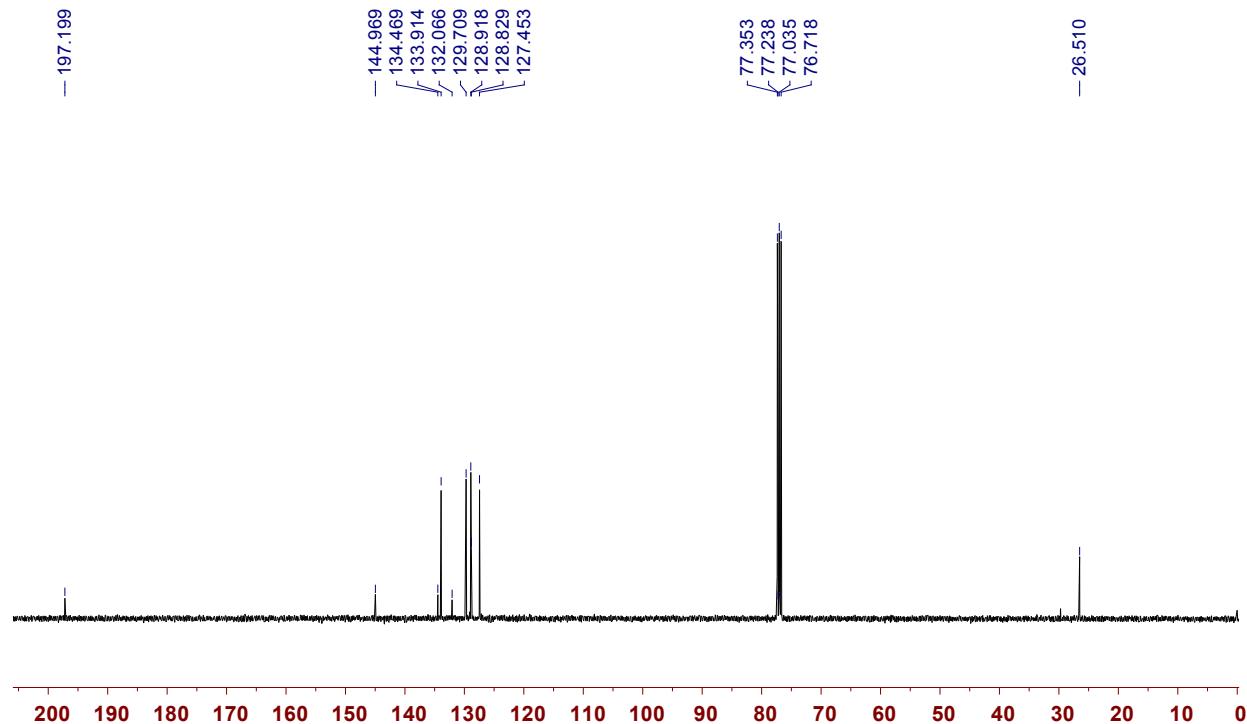


Fig. S38. ^{13}C NMR spectrum of compound **6a** in CDCl_3

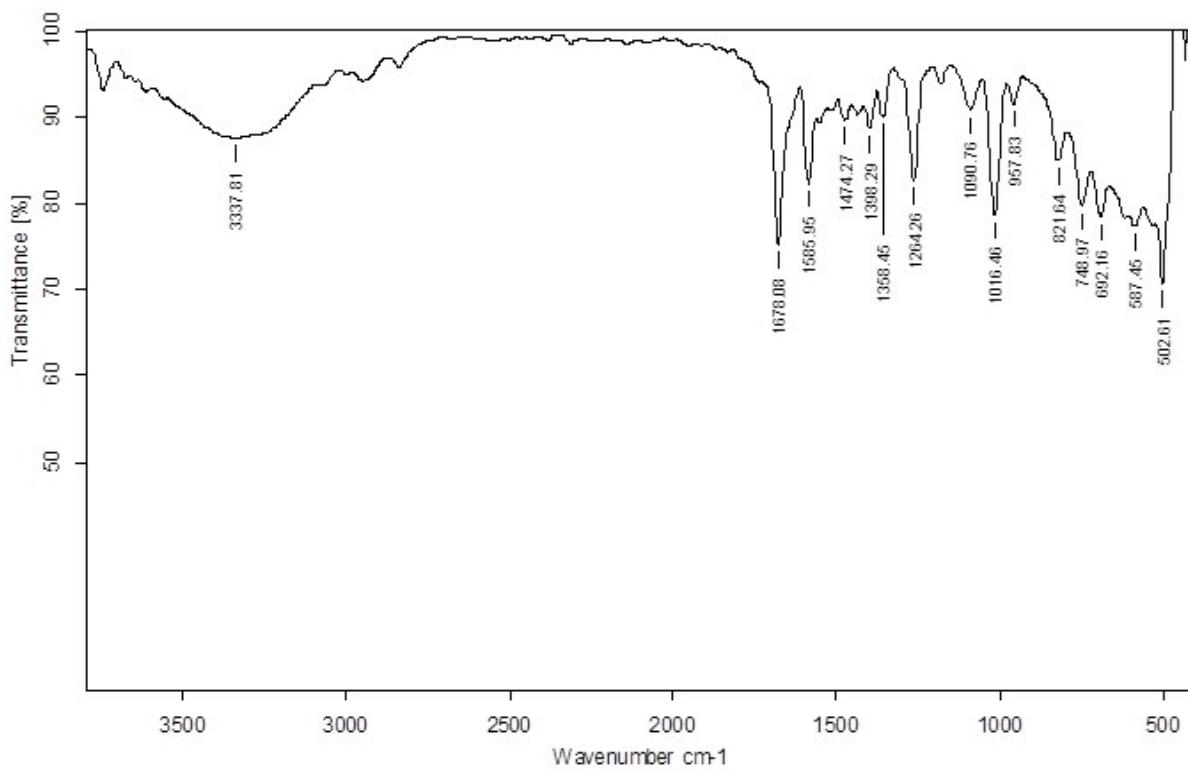


Fig. S39. Neat FT-IR spectrum of complex **6a**

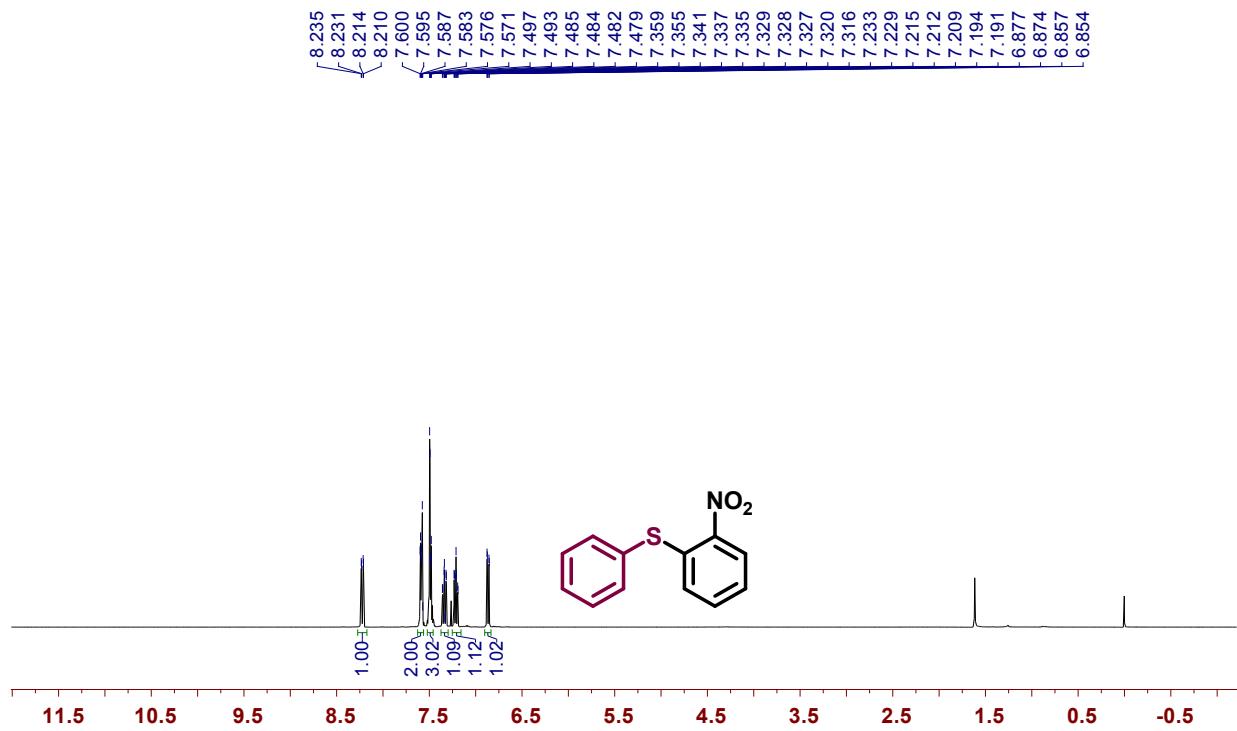


Fig. S40. ^1H NMR spectrum of compound **7a** in CDCl_3

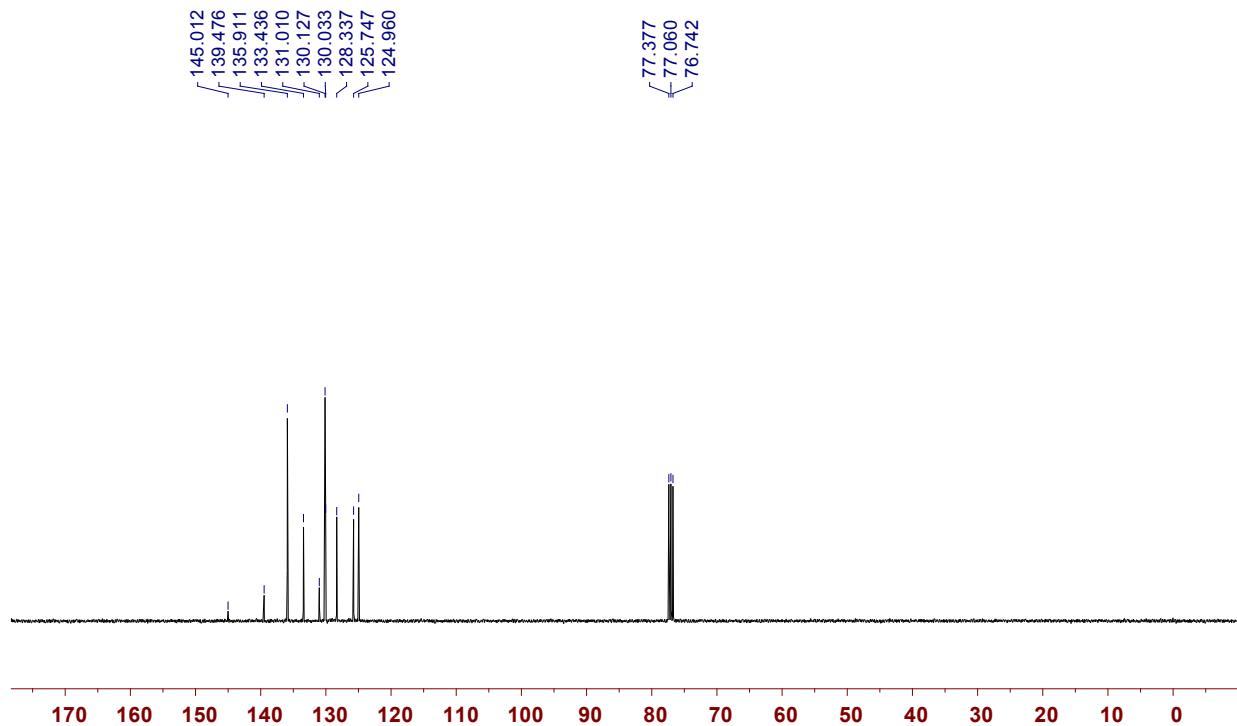


Fig. S41. ^{13}C NMR spectrum of compound **7a** in CDCl_3

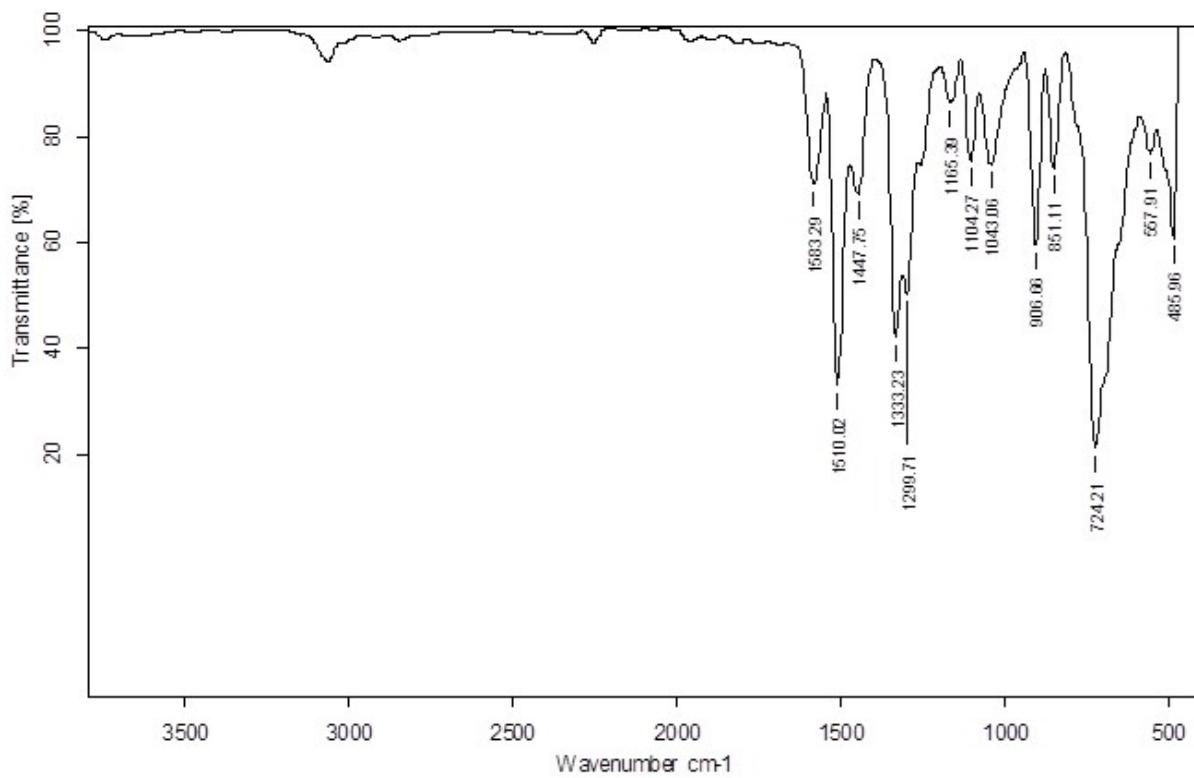


Fig. S42. Neat FT-IR spectrum of complex **7a**

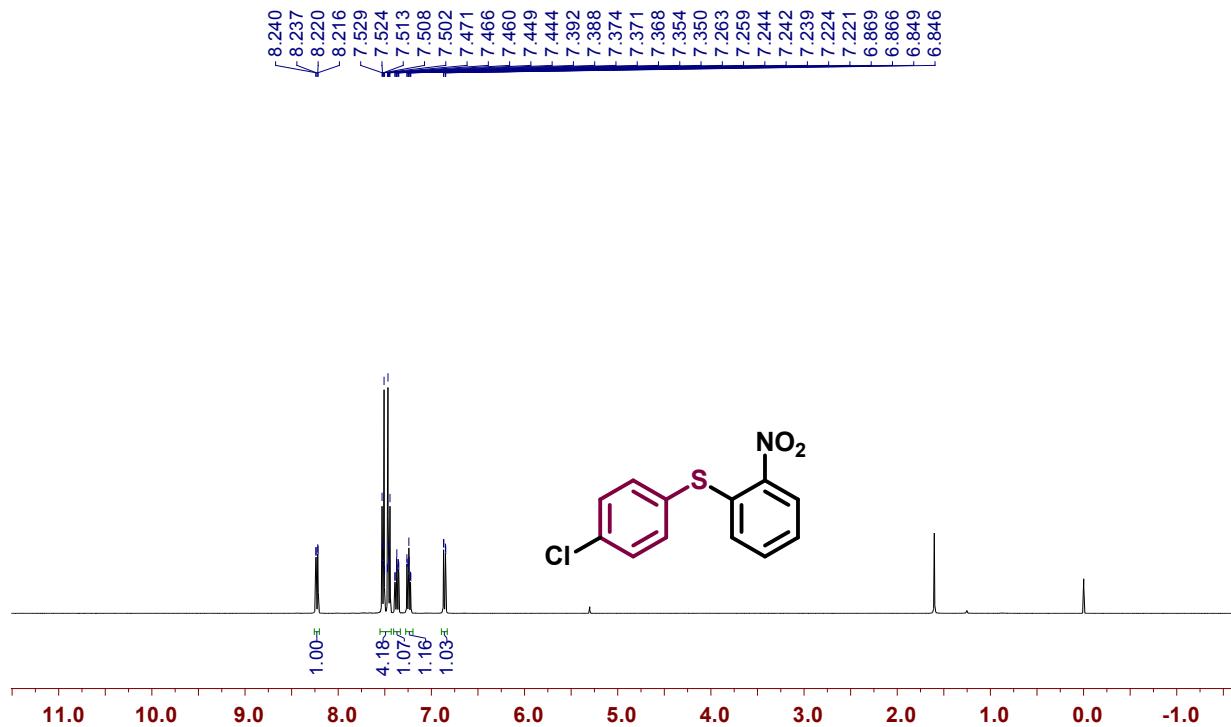


Fig. S43. ^1H NMR spectrum of compound **8a** in CDCl_3

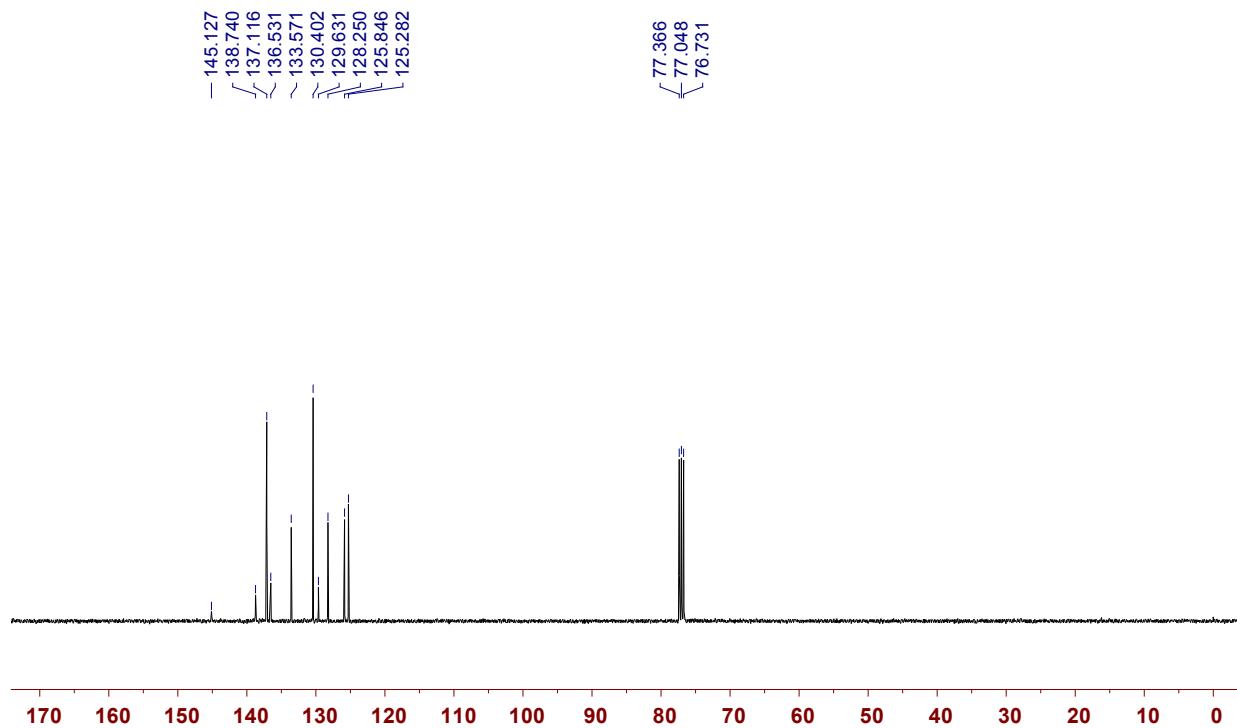


Fig. S44. ^{13}C NMR spectrum of compound **8a** in CDCl_3

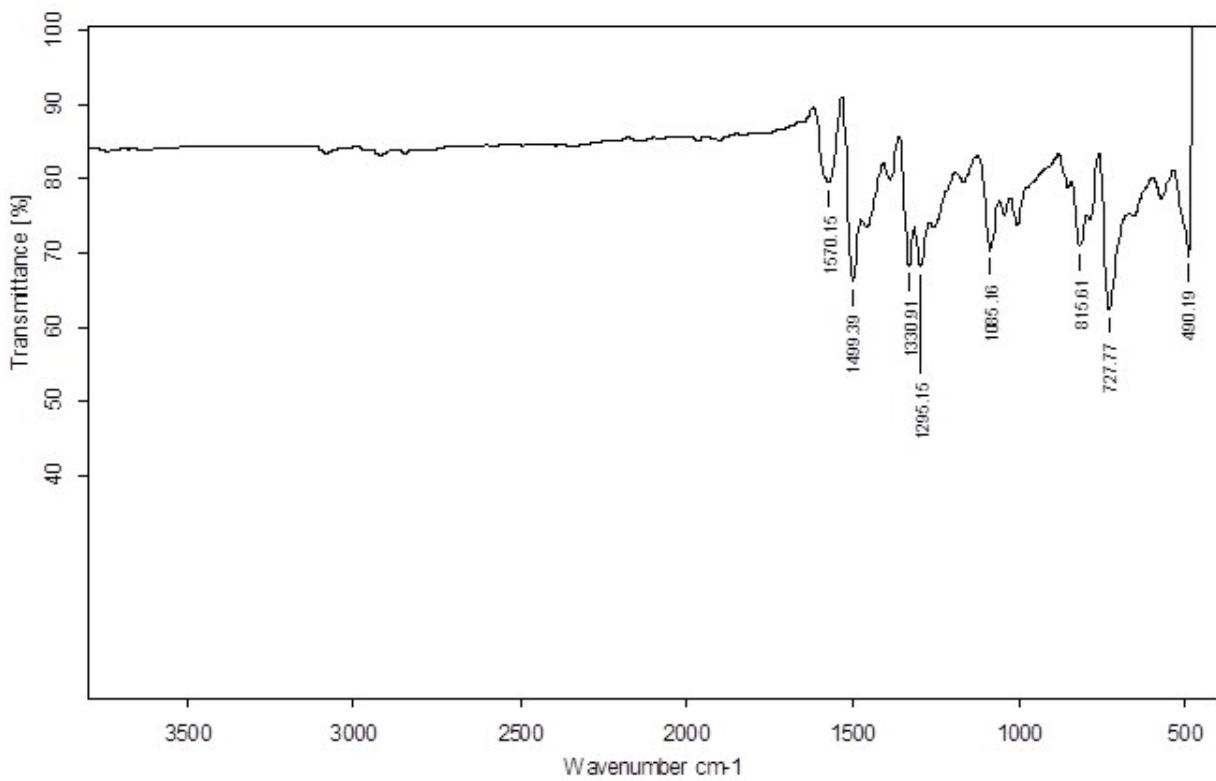


Fig. S45. Neat FT-IR spectrum of complex **8a**

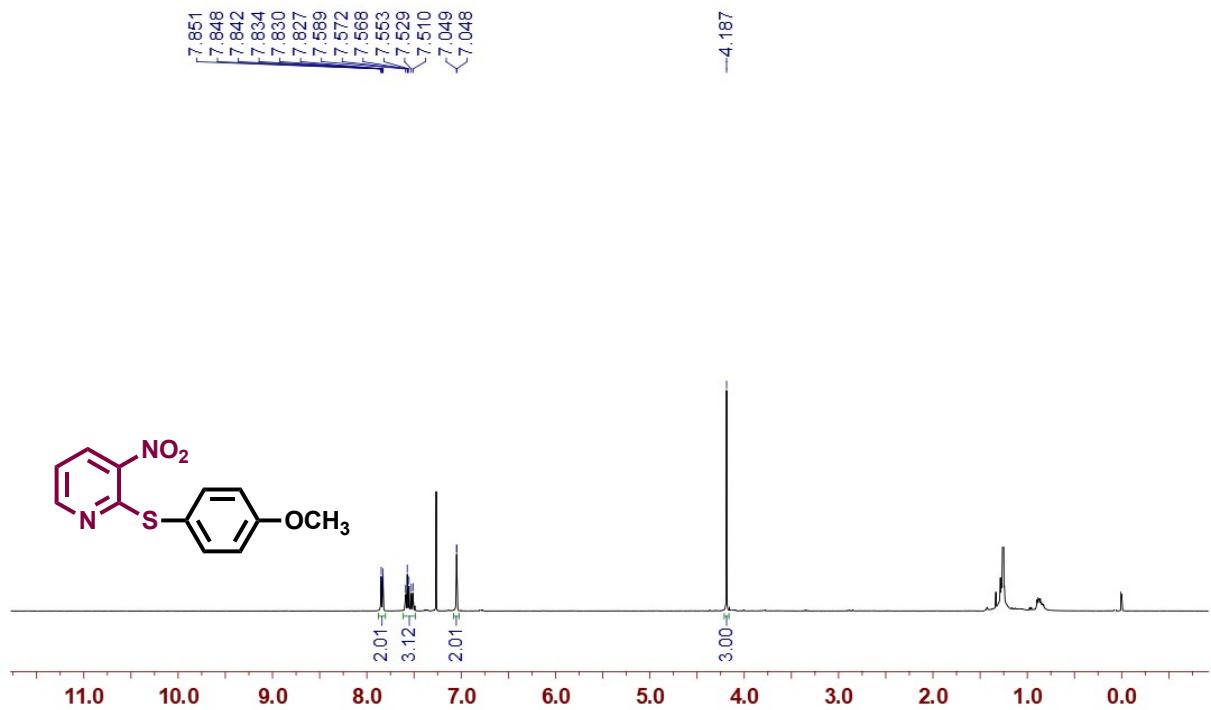


Fig. S46. ^1H NMR spectrum of compound 9a in CDCl_3

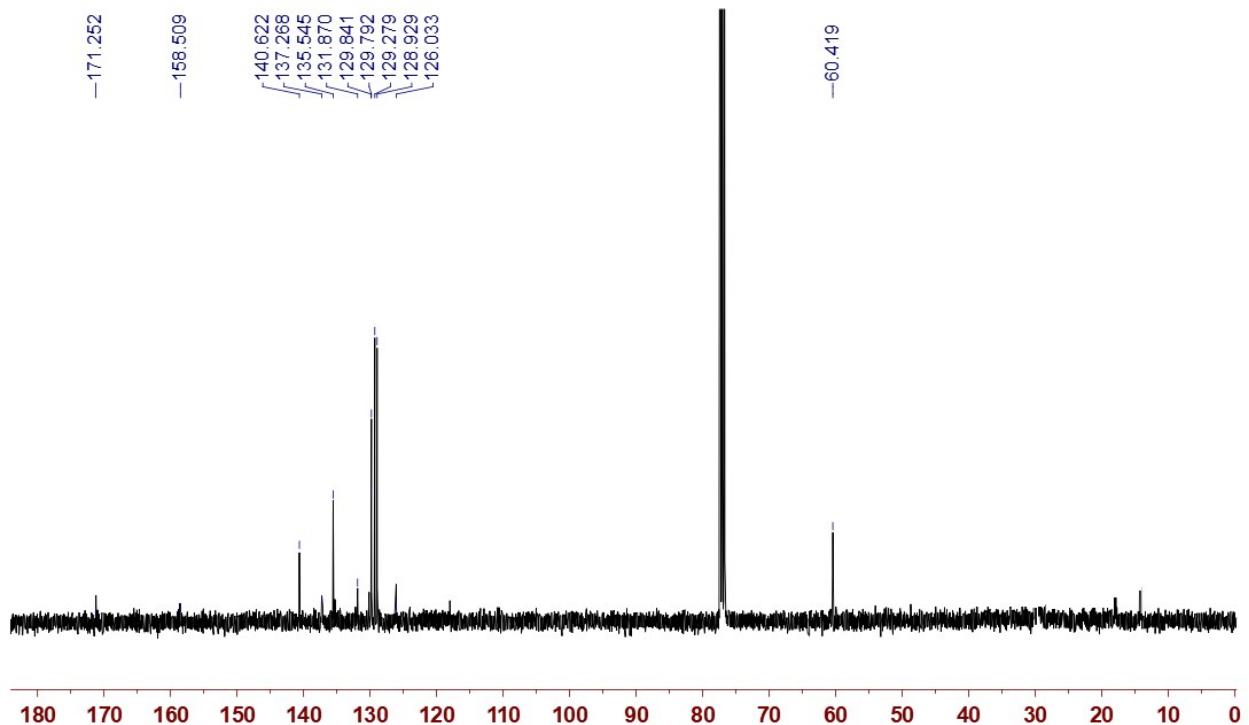


Fig. S47. ^{13}C NMR spectrum of compound 9a in CDCl_3

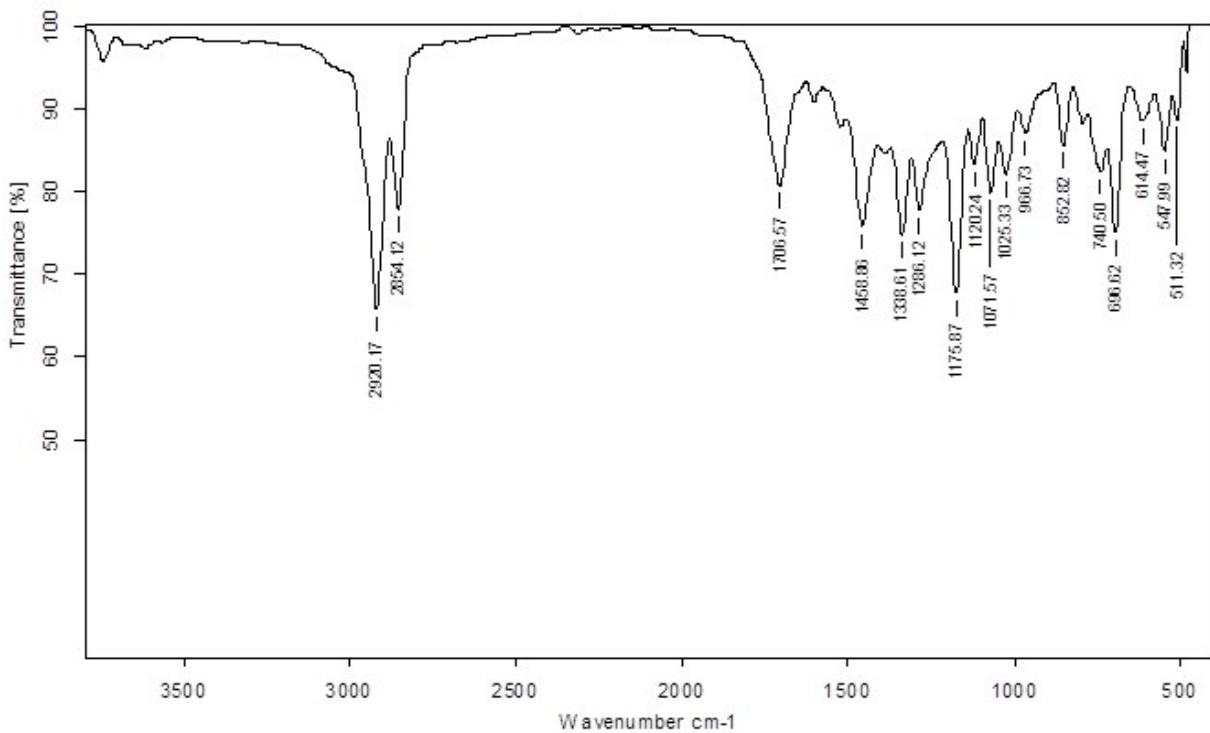


Fig. S48. Neat FT-IR spectrum of complex **9a**

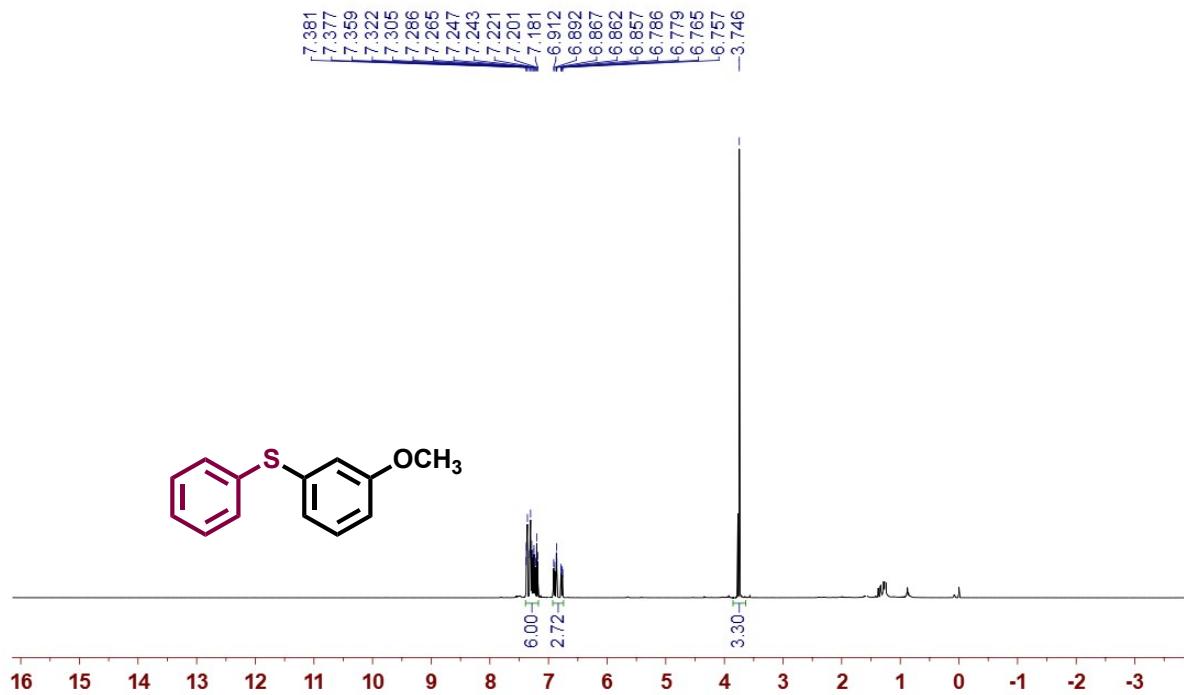


Fig. S49. ^1H NMR spectrum of compound **10a** in CDCl_3

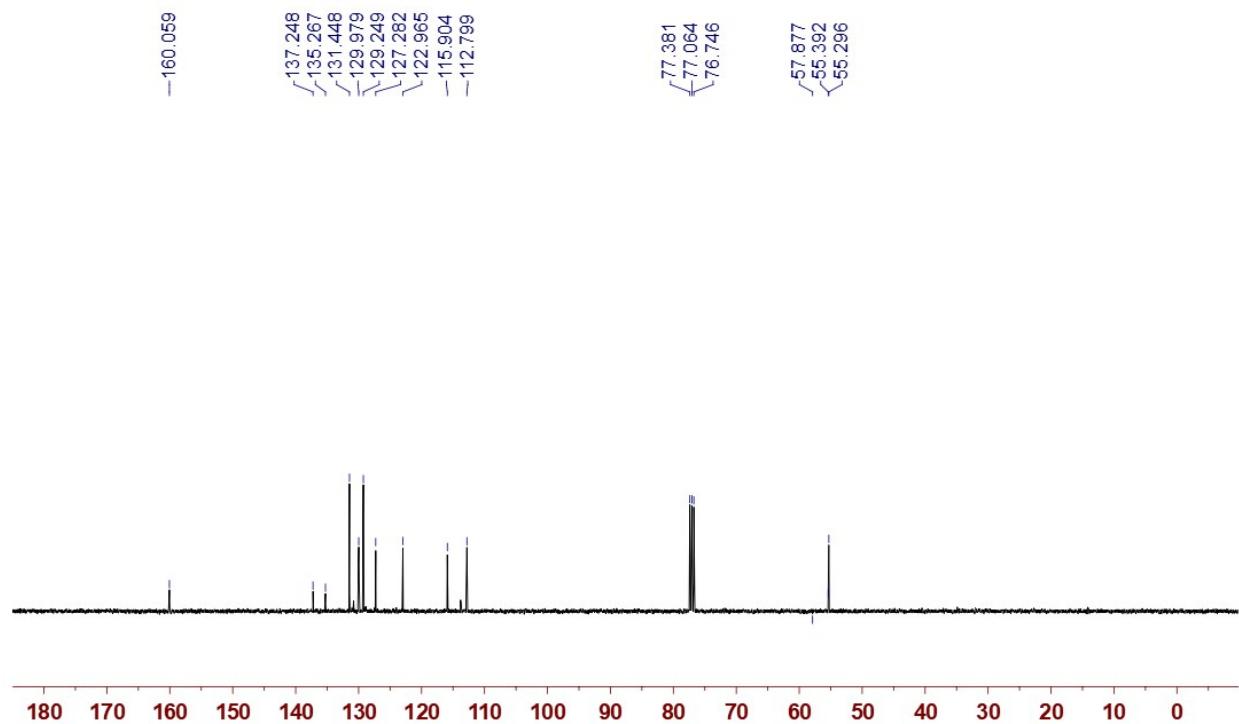


Fig. S50. ^{13}C NMR spectrum of compound **10a** in CDCl_3

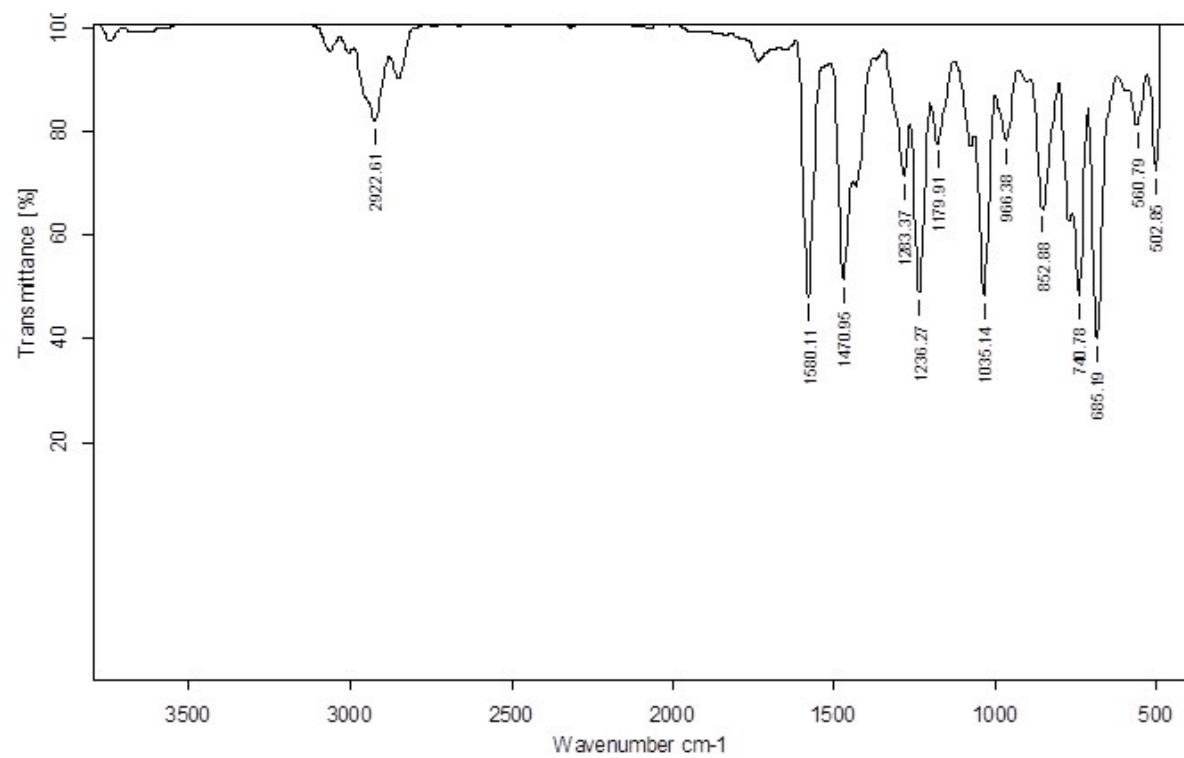


Fig. S51. Neat FT-IR spectrum of complex **10a**

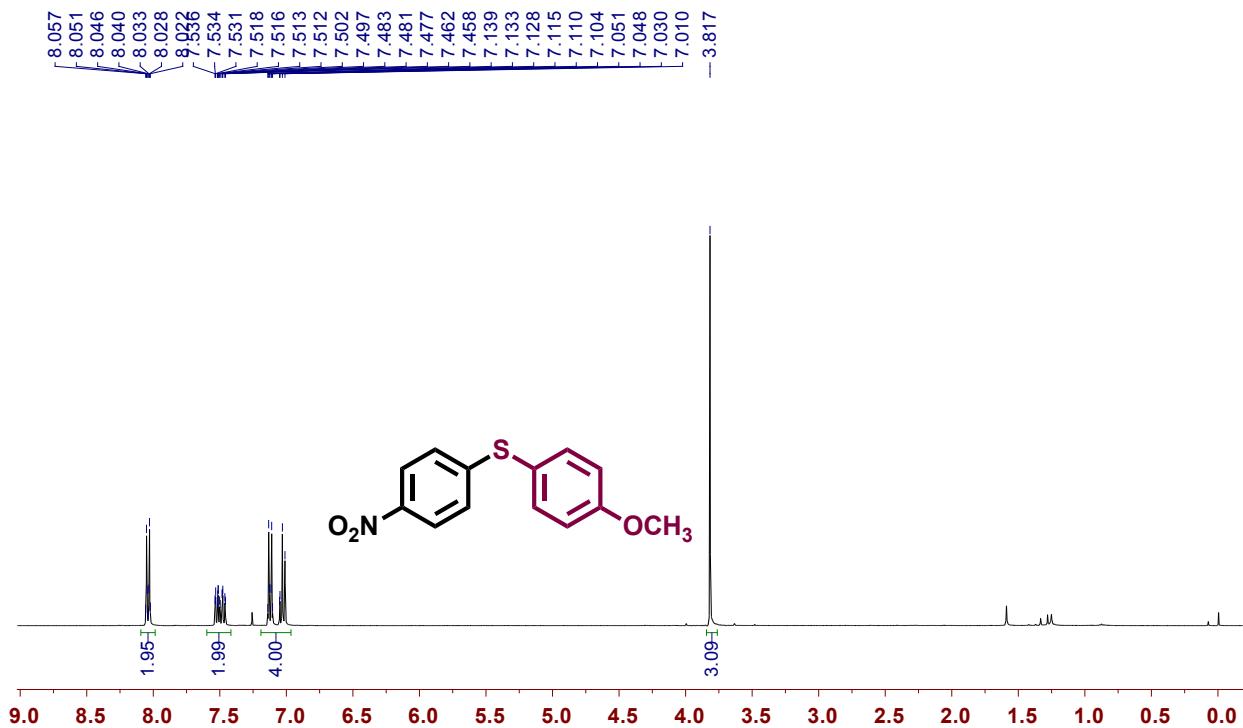


Fig. S52. ^1H NMR spectrum of compound **11a** in CDCl_3

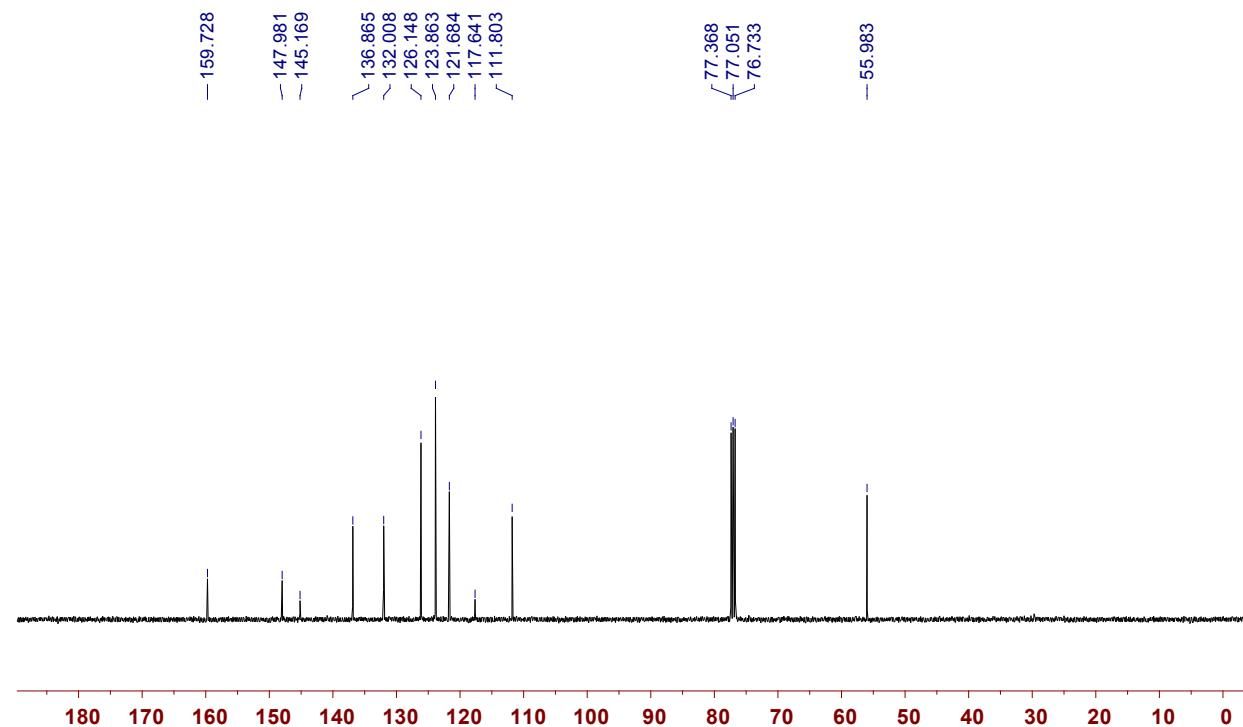


Fig. S53. ^{13}C NMR spectrum of compound **11a** in CDCl_3

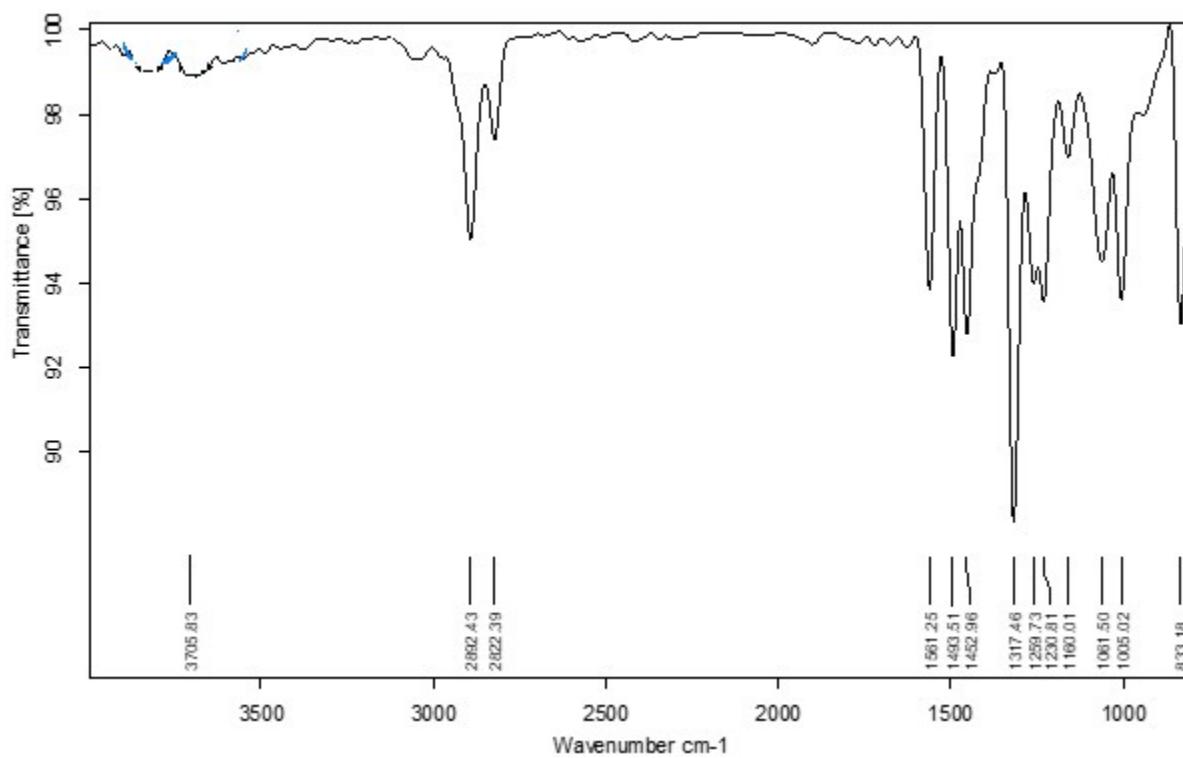


Fig. S54. Neat FT-IR spectrum of complex **11a**

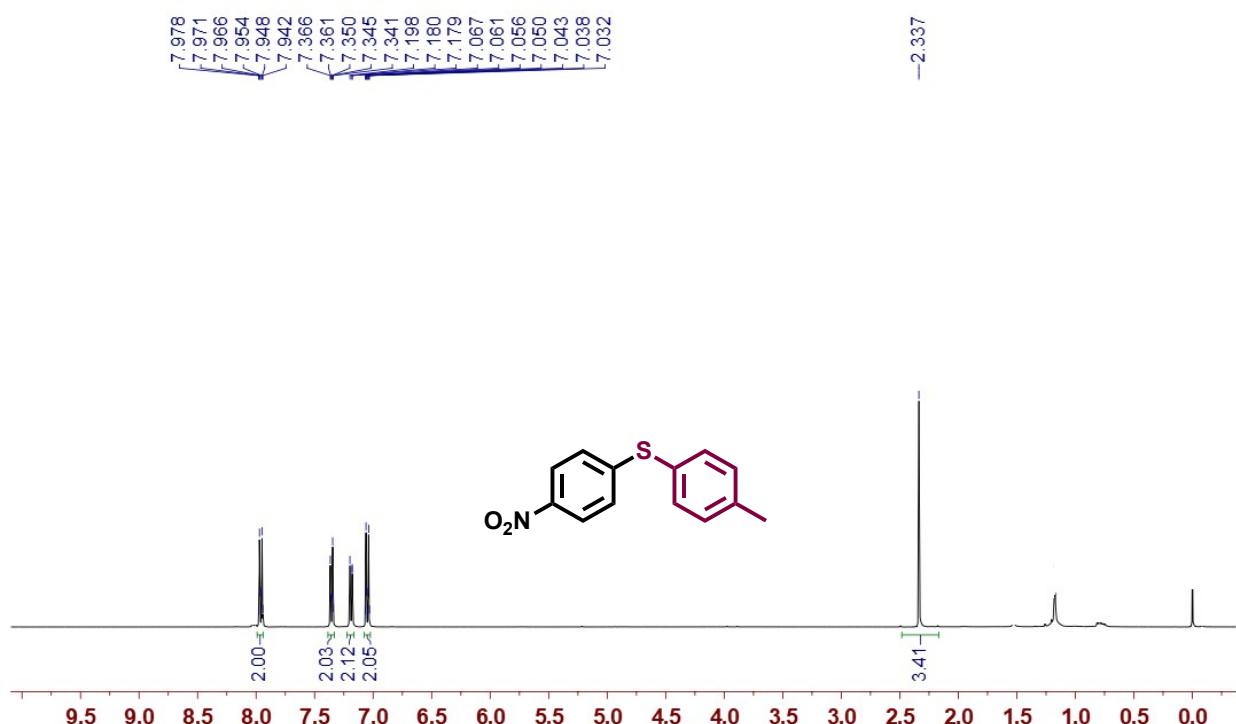


Fig. S55. ^1H NMR spectrum of compound **12a** in CDCl_3

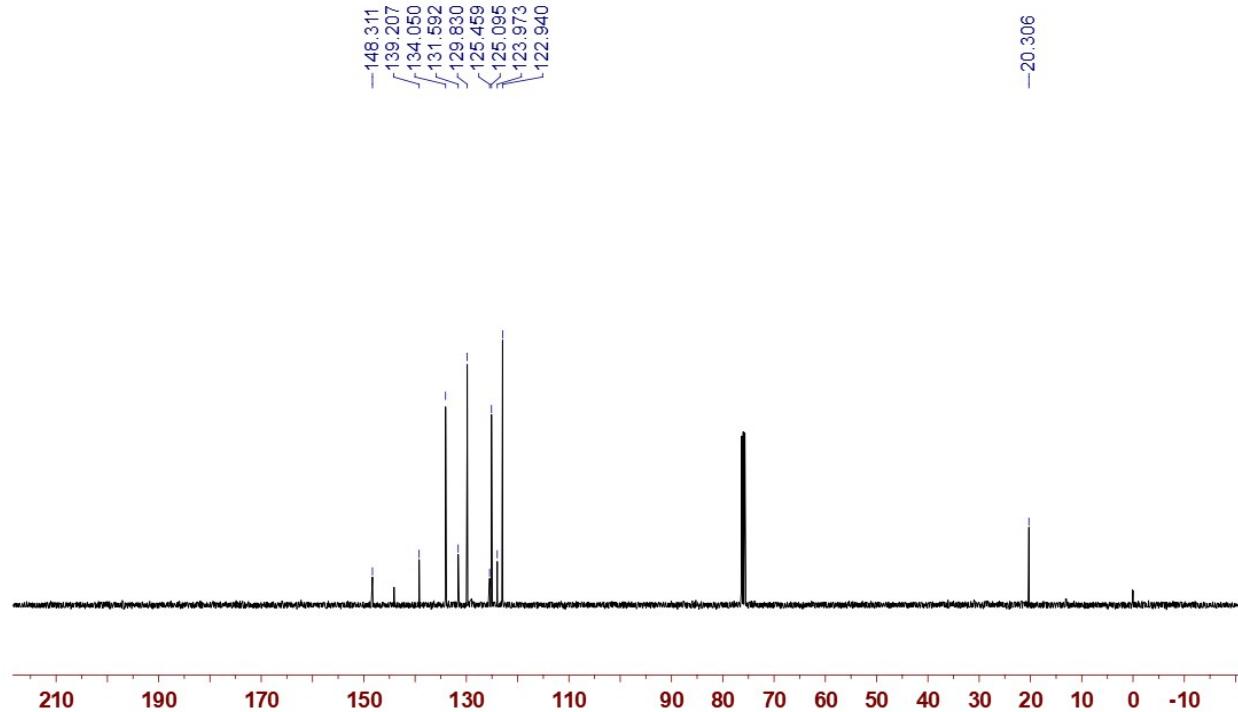


Fig. S56. ^{13}C NMR spectrum of compound **12a** in CDCl_3

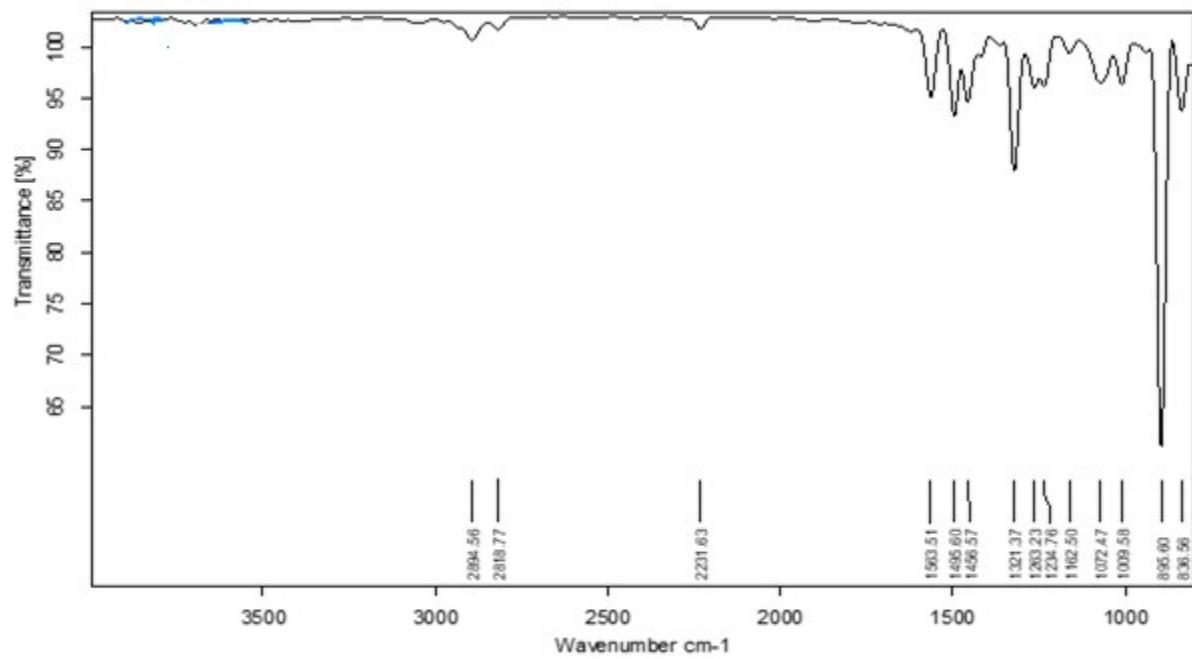


Fig. S57. Neat FT-IR spectrum of complex **12a**

Table S1: Solid state structural parameters of **1-4**

	1	2	3	4
Empirical formula	C ₃₀ H ₂₈ N ₄ Se ₂ Cl ₂ Zn	C ₃₀ H ₂₈ N ₄ Se ₂ Br ₂ Zn	C ₂₈ H ₄₈ N ₈ Se ₄ F ₈ B ₂ Zn	C ₂₈ H ₄₈ N ₈ Se ₄ O ₈ Cl ₂ Zn
Formula weight	737.93	827.68	1089.61	1072.85
Temperature (K)	293	293	293	293
Crystal system	Triclinic	Triclinic	Tetragonal	Triclinic
Space group	P1	P-1	I41/a	P-1
<i>a</i> /Å	8.2138(4)	8.3550(7)	12.4234(2)	12.6182(9)
<i>b</i> /Å	11.5106(6)	11.5840(8)	12.4234(2)	12.6356(9)
<i>c</i> /Å	16.2370(9)	16.3071(11)	27.7432(11)	15.6832(12)
α°	93.013(4)	92.900(6)	90	67.891(7)
β°	96.577(4)	96.600(6)	90	68.825(7)
γ°	93.489(4)	92.887(6)	90	89.725(6)
Volume (Å ³)	1519.45(13)	1563.3(2)	4281.9(2)	2135.2(3)
<i>Z</i>	4	4	4	2
$\rho_{\text{calc}}/\text{mg mm}^{-3}$	1.6114	1.7583	1.6901	1.6686
Absorption coefficient (μ/mm^{-1})	5.684	6.947	5.351	6.28
<i>F</i> (000)	729.5	800.3	2139.0	1058.3
Reflections collected	10642	9043	4375	8035
<i>R</i> _{int}	0.0231	0.0419	0.0185	0.0249
GOF on <i>F</i> ²	1.073	1.183	1.041	1.062
<i>R</i> ₁ (<i>I</i> >2σ(<i>I</i>))	0.0302	0.0691	0.0536	0.0780
w <i>R</i> ₂ (<i>I</i> >2σ(<i>I</i>))	0.0780	0.2163	0.1478	0.2084
<i>R</i> ₁ values (all data)	0.0358	0.0975	0.0695	0.0953
<i>R</i> ₂ values (all data)	0.0841	0.3001	0.1735	0.2522

Table S2: Solid state structural parameters of **5**

	5
Empirical formula	C ₁₄ H ₃₀ N ₄ Se ₂ Br ₂ Zn
Formula weight	631.48
Temperature (K)	293
Crystal system	Orthorhombic
Space group	Pbca
<i>a</i> /Å	14.3427(6)
<i>b</i> /Å	14.0781(5)
<i>c</i> /Å	21.6645(8)
$\alpha/^\circ$	90
$\beta/^\circ$	90
$\gamma/^\circ$	90
Volume (Å ³)	4374.5(3)
<i>Z</i>	4
ρ_{calc} /mg mm ⁻³	1.9167
Absorption coefficient (μ/mm^{-1})	9.667
<i>F</i> (000)	2399.1
Reflections collected	9953
<i>R</i> _{int}	0.0388
GOF on <i>F</i> ²	1.662
<i>R</i> ₁ (<i>I</i> >2σ(<i>I</i>))	0.1307
w <i>R</i> ₂ (<i>I</i> >2σ(<i>I</i>))	0.3611
<i>R</i> ₁ values (all data)	0.1694
<i>R</i> ₂ values (all data)	0.4641

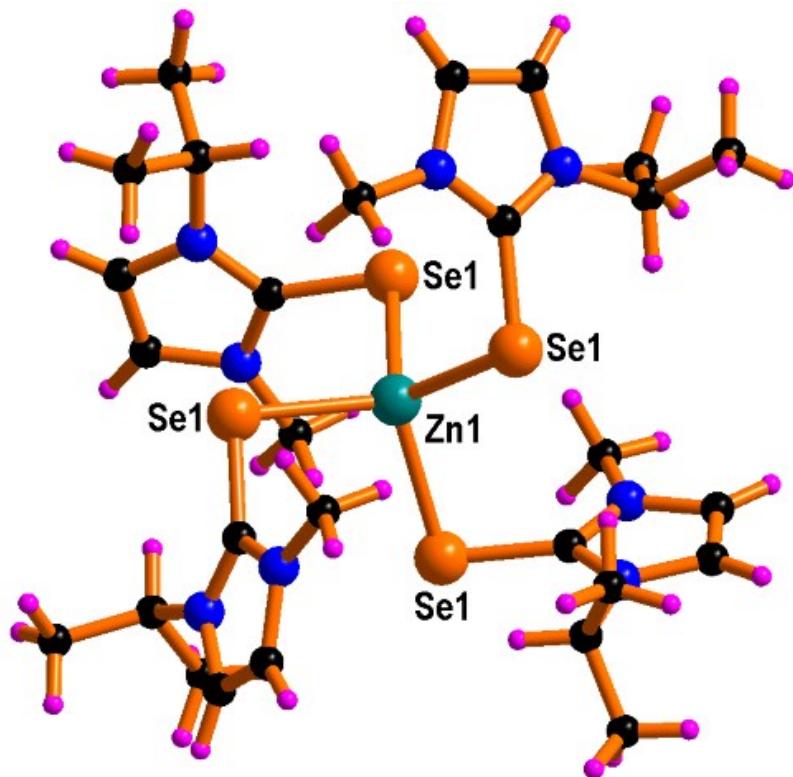


Fig. S58. The solid state structure of **3**. The disordered BF_4^- anions are omitted for clarity. Selected bond lengths (\AA) and bond angles ($^\circ$): Zn(1)-Se(1) 2.471(6), Se(1)-Zn(1)-Se(2) 104.86(14), Se(1)-Zn(1)-Se(3) 104.86.

DFT Calculation^[1,2]

Table S3: Imidazolydene

Bond orbital	Occupancy	Coefficients		Hybrids
n_{N3}	0.78660			s(0.00%)p 1.00(100.00%)
n_{C4}	0.96230			s(53.09%)p 0.88(46.91%)
n^*_{C4}	0.32839			s(0.00%)p 1.00(100.00%)
n_{N5}	0.78398			s(0.00%)p 1.00(100.00%)
π^*_{C1-C2}	0.13546	49.74%	0.7052*C1	s(0.00%)p 1.00(100.00%)
		50.26%	-0.7090*C2	s(0.00%)p 1.00(100.00%)
σ^*_{C1-N5}	0.02234	62.88%	0.7930*C1	s(26.83%)p 2.73(73.17%)
		37.12%	-0.6092*N5	s(31.93%)p 2.13(68.07%)

Table S4: Imidazolydene

Donor	Acceptor	ΔE kcal/mol	$E_{\text{donor}} - E_{\text{acceptor}}$ a.u.	$F(i,j)$ a.u.
n_{N3}	n^*_{C4}	44.76	0.19	0.125
n_{N3}	π^*_{C1-C2}	16.01	0.27	0.086
n_{N5}	n^*_{C4}	44.82	0.19	0.125
n_{N5}	π^*_{C1-C2}	15.80	0.27	0.085
n_{C4}	σ^*_{C1-N5}	4.01	0.67	0.066
n_{C4}	σ^*_{C2-N3}	3.96	0.68	0.066

Table S5: Imidazathione

Bond orbital	Occupancy	Coefficients		Hybrids
n_{N3}	0.78766			s(0.00%)p 1.00(100.00%)
n^*_{C4}	0.49293			s(0.00%)p 1.00(100.00%)
n_{N5}	0.78766			s(0.00%)p 1.00(100.00%)
n^1_{S8}	0.93873			s(0.00%)p 1.00(100.00%)
n^2_{S8}	0.82259			s(0.00%)p 1.00(100.00%)
π^*_{C1-C2}	0.13512	50.00%	0.7071*C1	s(0.00%)p 1.00(100.00%)
		50.00%	-0.7071*C2	s(0.00%)p 1.00(100.00%)
σ^*_{N3-C4}	0.03428	36.48%	0.6040* 3	s(34.01%)p 1.94(65.99%)
		63.52%	-0.7970*C4	s(29.98%)p 2.34(70.02%)
σ^*_{C4-N5}	0.03428	63.52%	0.7970*C4	s(29.98%)p 2.34(70.02%)
		36.48%	-0.6040*N5	s(34.01%)p 1.94(65.99%)

Table S6: Imidazathione

Donor	Acceptor	ΔE kcal/mol	$E_{\text{donor}} - E_{\text{acceptor}}$ a.u.	$F(i,j)$ a.u.
n_{N3}	π^*_{C1-C2}	15.98	0.27	0.086
n_{N5}	n^*_{C4}	63.13	0.11	0.126
n_{N5}	π^*_{C1-C2}	15.98	0.27	0.086
n_{S8}	σ^*_{N3-C4}	6.08	0.57	0.076
n_{S8}	σ^*_{C4-N5}	6.08	0.57	0.076
n_{S8}	n^*_{C4}	208.53	0.02	0.096

Table S7: Imidazaselone

Bond orbital	Occupancy	Coefficients		Hybrids
n_{N3}	0.78415			s(0.00%)p 1.00(100.00%)
n^*_{C4}	0.49199			s(0.00%)p 1.00(100.00%)
n_{N5}	0.78415			s(0.00%)p 1.00(100.00%)
n_{Se16}	0.94484			s(0.00%)p 1.00(99.99%) d0.00(0.01%)
π^*_{C1-C2}	0.13537	50.00%	0.7071*C1	s(0.00%)p 1.00(100.00%)
		50.00%	-0.7071*C2	s(0.00%)p 1.00(100.00%)
σ^*_{N3-C4}	0.03164	36.09%	0.6007*N3	s(34.33%)p 1.91(65.67%)
		63.91%	-0.7995*C4	s(29.69%)p 2.37(70.31%)
σ^*_{C4-N5}	0.03164	63.91%	0.7995*C4	s(29.69%)p 2.37(70.31%)
		36.09%	-0.6007*N5	s(34.33%)p 1.91(65.67%)

Table S8: Imidazaselone

Donor	Acceptor	ΔE kcal/mol	$E_{\text{donor}} - E_{\text{acceptor}}$ a.u.	$F(i,j)$ a.u.
n_{N3}	n^*_{C4}	62.08	0.12	0.126
n_{N3}	π^*_{C1-C2}	15.97	0.27	0.086
n_{N5}	n^*_{C4}	62.08	0.12	0.126
n_{N5}	π^*_{C1-C2}	15.97	0.27	0.086
n_{Se16}	σ^*_{N3-C4}	4.98	0.56	0.068
n_{Se16}	σ^*_{C4-N5}	4.98	0.56	0.068

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- 1) Gaussian 16 Revision A.03 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, R. G. Janesko, R. Gomber, R. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams, F. Ding, F. Liannarini, F. Egidi, J. Goings, R. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakai, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Hevd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
- 2) GaussView, Version 6, R. Dennington, T. A. Keith, and J. M. Millam, Semichem Inc., Shawnee Mission, KS, 2016.