

One-pot Synthesis of unsubstituted- and methyl substituted-Pyrazinyl Diselenides and Monoselenides: Structural, Optical Property Characterization and DFT Calculations

Nisha Kushwah,^{a*} Suresh Chopade,^a Amey Wadawale,^a P. B. Sharma^a and G. Kedarnath^{a,b*}

Scheme 1 Synthesis of methyl substituted-dipyrazinyldiselenide and -monoselenide with numbering.

Fig S1. IR spectra of Bis(2-pyrazinyl)selenide [(2-pyz)₂Se] (**1**)

Fig S2. IR spectra of Bis(2-pyrazinyl)diselenide [(2-pyzSe)₂] (**2**)

Fig S3. IR spectra of Bis(2,5-dimethyl-3-pyrazinyl)selenide [(2,5-Me₂-3-pyz)₂Se] (**3**)

Fig S4. IR spectra of Bis(2,5-dimethyl-3-pyrazinyl)diselenide [(2,5-Me₂-3-pyzSe)₂] (**4**)

Fig S5. ¹H NMR spectra of bis(2-pyrazinyl)selenide [(2-pyz)₂Se] (**1**)

Fig S6. ¹³C{¹H} NMR spectra of Bis(2-pyrazinyl)selenide [(2-pyz)₂Se] (**1**)

Fig S7. ⁷⁷Se{¹H} NMR spectra of Bis(2-pyrazinyl)selenide [(2-pyz)₂Se] (**1**)

Fig S8. ¹H NMR spectra of Bis(2-pyrazinyl)diselenide [(2-pyzSe)₂] (**2**)

Fig S9. ¹³C{¹H} NMR spectra of bis(2-pyrazinyl)diselenide [(2-pyzSe)₂] (**2**)

Fig S10. ⁷⁷Se{¹H} NMR spectra of bis(2-pyrazinyl)diselenide [(2-pyzSe)₂] (**2**)

Fig S11. ¹H NMR spectra of bis(2,5-dimethyl-3-pyrazinyl)selenide [(2,5-Me₂-3-pyz)₂Se] (**3**)

Fig S12. ¹³C{¹H} NMR spectra of Bis(2,5-dimethyl-3-pyrazinyl)selenide [(2,5-Me₂-3-pyz)₂Se] (**3**)

Fig S13. ⁷⁷Se{¹H} NMR spectra of Bis(2,5-dimethyl-3-pyrazinyl)selenide [(2,5-Me₂-3-pyz)₂Se]

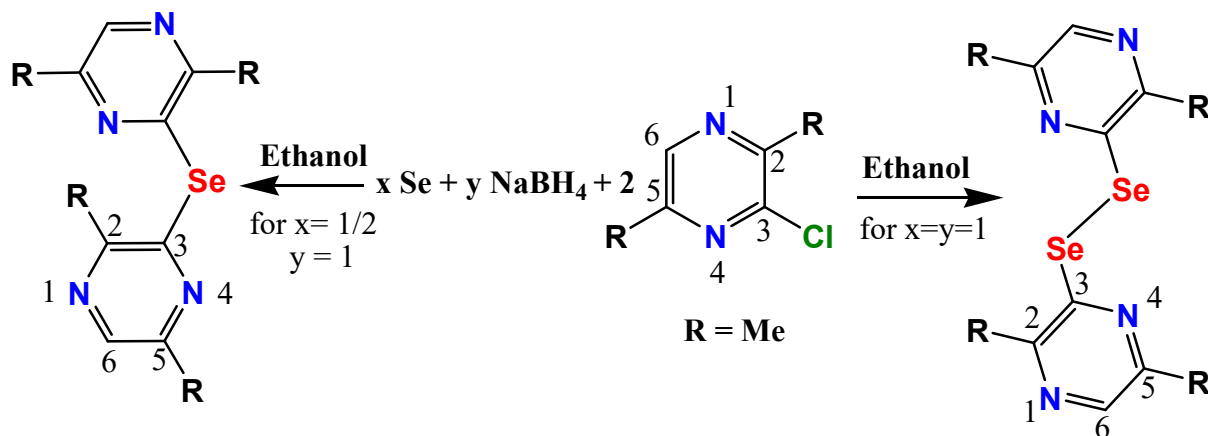
Fig S14. ¹H NMR spectra of Bis(2,5-dimethyl-3-pyrazinyl)diselenide [(2,5-Me₂-3-pyzSe)₂] (**4**)

Fig S15. ¹³C{¹H} NMR spectra of Bis(2,5-dimethyl-3-pyrazinyl)diselenide [(2,5-Me₂-3-pyzSe)₂] (**4**)

Fig S16. ⁷⁷Se{¹H} NMR spectra of Bis(2,5-dimethyl-3-pyrazinyl)diselenide [(2,5-Me₂-3-pyzSe)₂] (**4**)

Fig S17: Absorption-, excitation-, emission-spectra of [(3-Me-2-pySe)₂].

Fig S18: Absorption-, excitation-, emission-spectra of [(4,6-Me₂-2-pymSe)₂].



Scheme 1 Synthesis of methyl substituted-dipyrazinyldiselenide and -monoselenide with numbering.

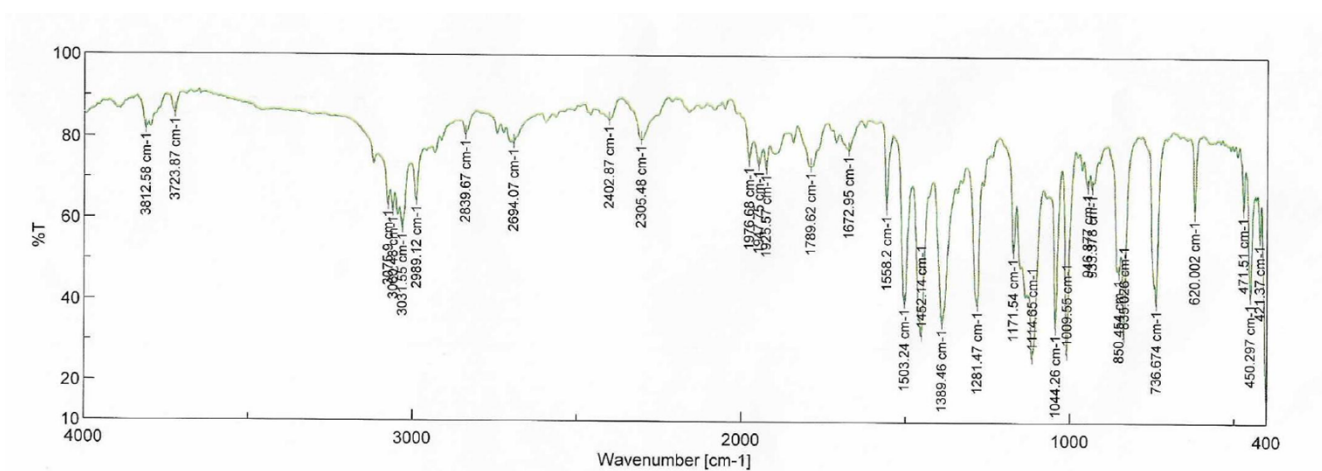


Fig S1: IR spectra of bis(2-pyrazinyl)selenide [(2-pyz)₂Se] (1)

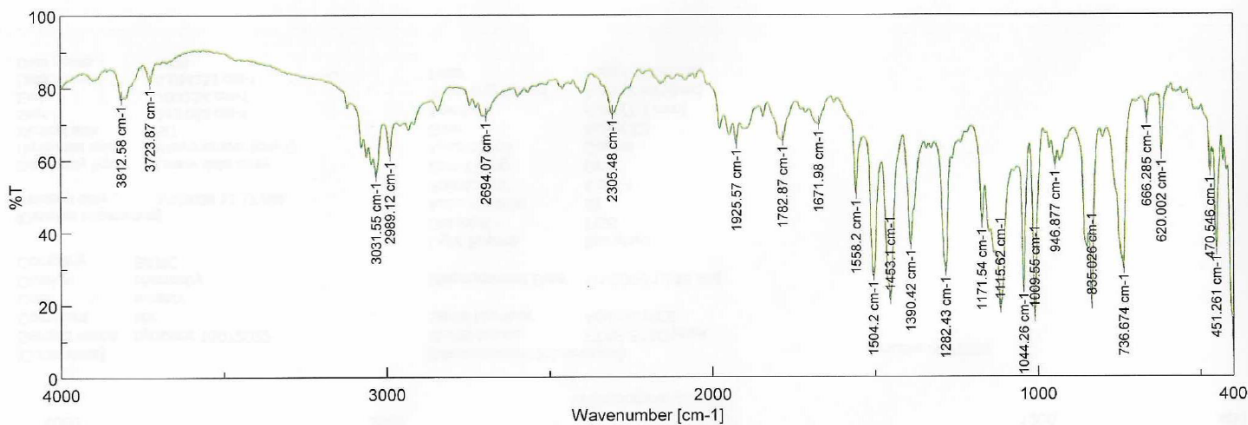


Fig S2: IR spectra of bis(2-pyrazinyl)diselenide [(2-pyzSe)₂] (2)

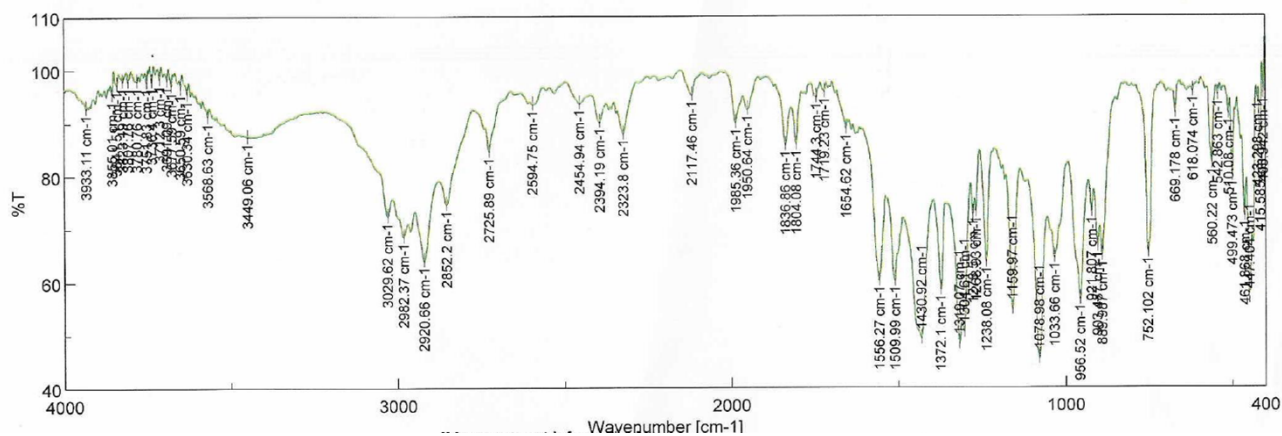


Fig S3: IR spectra of bis(2,5-dimethyl-3-pyrazinyl)selenide [(2,5-Me₂-3-pyz)₂Se] (3)

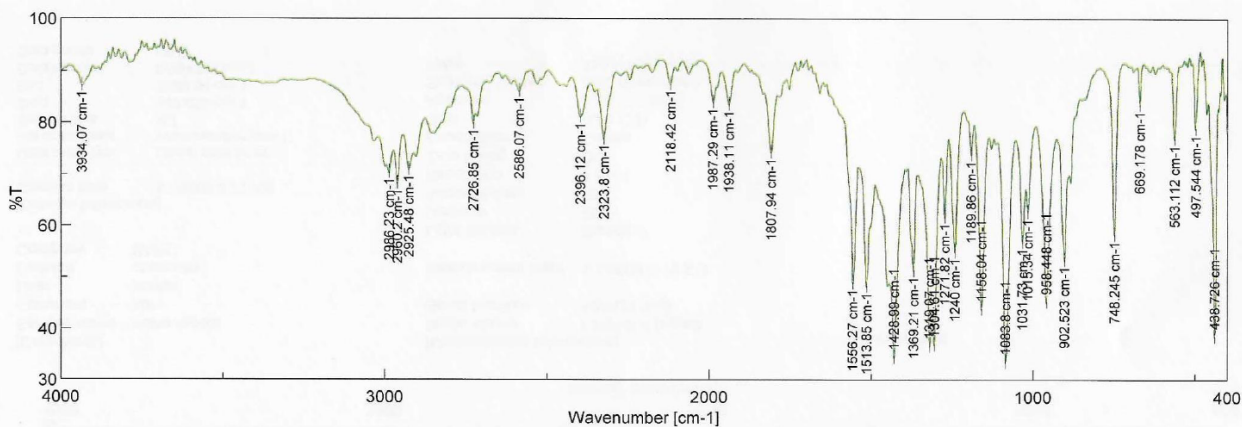


Fig S4: IR spectra of bis(2,5-dimethyl-3-pyrazinyl)diselenide [(2,5-Me₂-3-pyzSe)₂] (4)

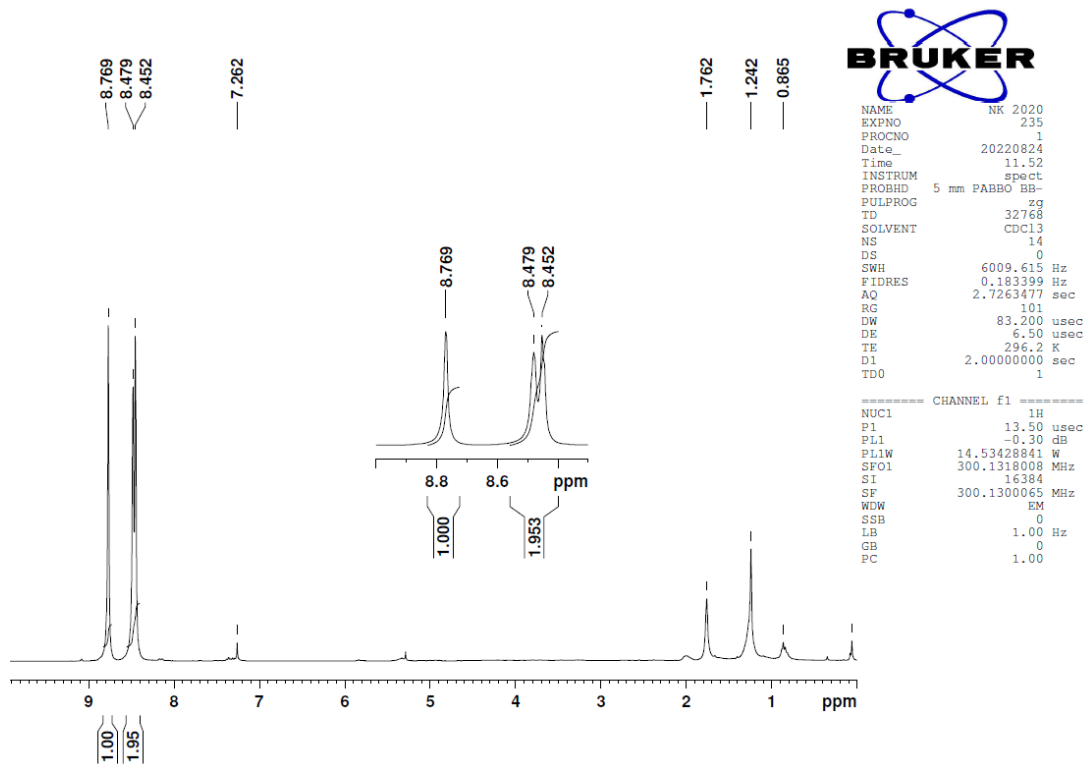


Fig S5: ^1H NMR spectra of bis(2-pyrazinyl)selenide [(2-pyz) $_2$ Se] (**1**)

(Peaks at 0.86, 1.24 and 1.74 is due to solvent residual signals) Ref: G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg *Organometallics* **29**(2010) 2176–2179.

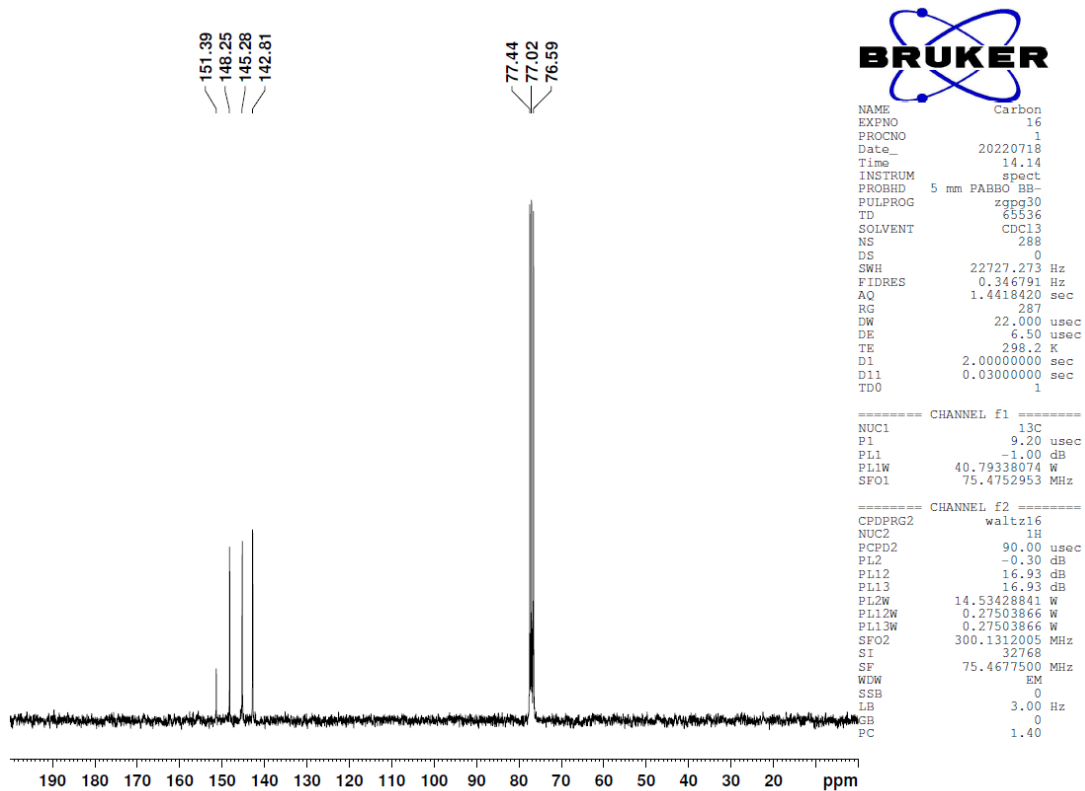


Fig S6: $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of Bis(2-pyrazinyl)selenide [(2-pyz) $_2$ Se] (1)

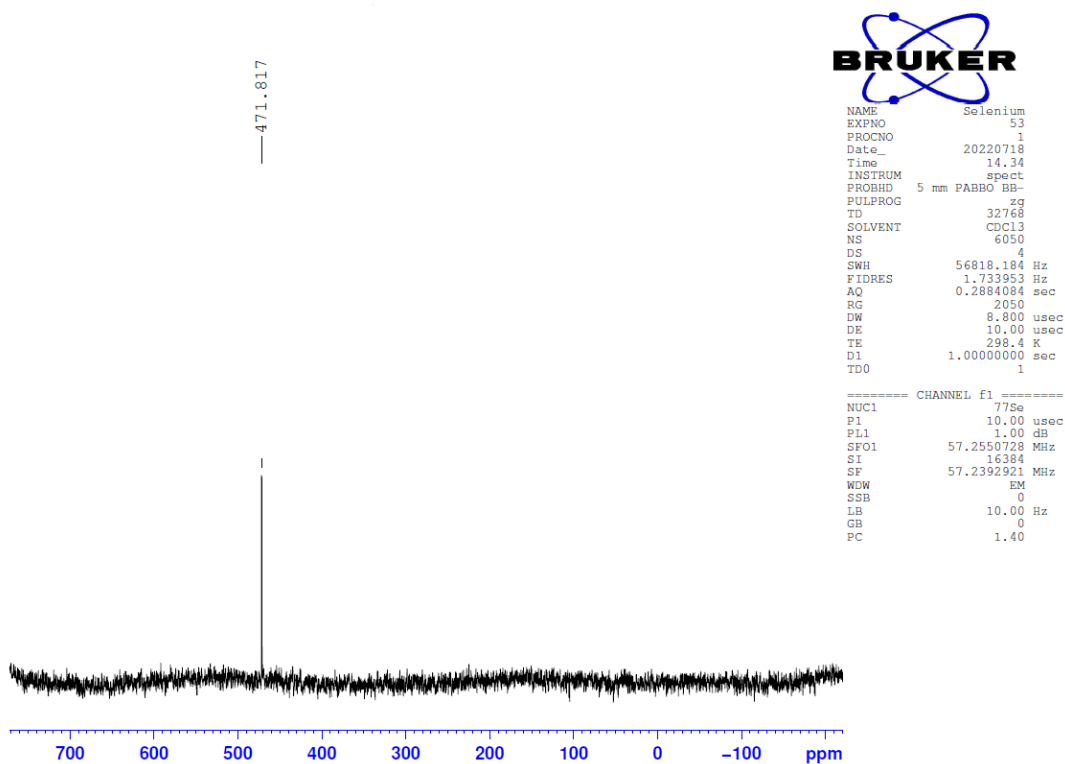


Fig S7: $^{77}\text{Se}\{^1\text{H}\}$ NMR spectra of bis(2-pyrazinyl)selenide [(2-pyz) $_2$ Se] (1)

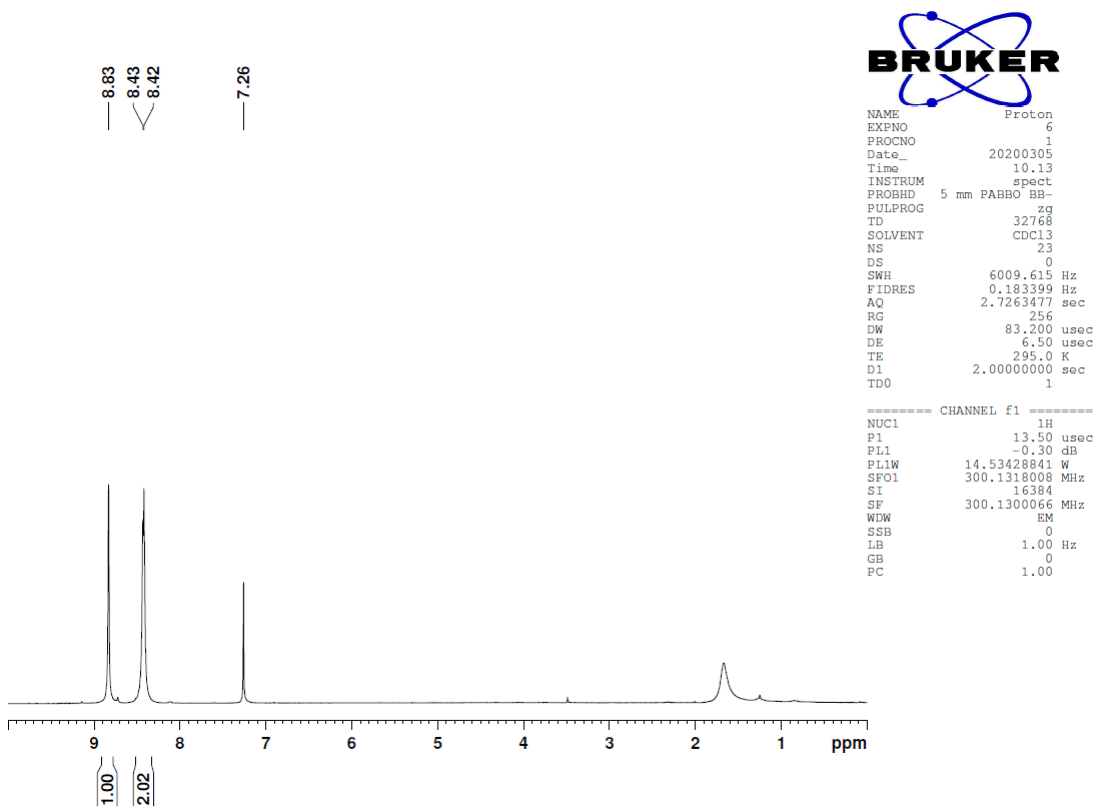


Fig S8: ^1H NMR spectra of bis(2-pyrazinyl)diselenide [(2-pyzSe) $_2$] (2)

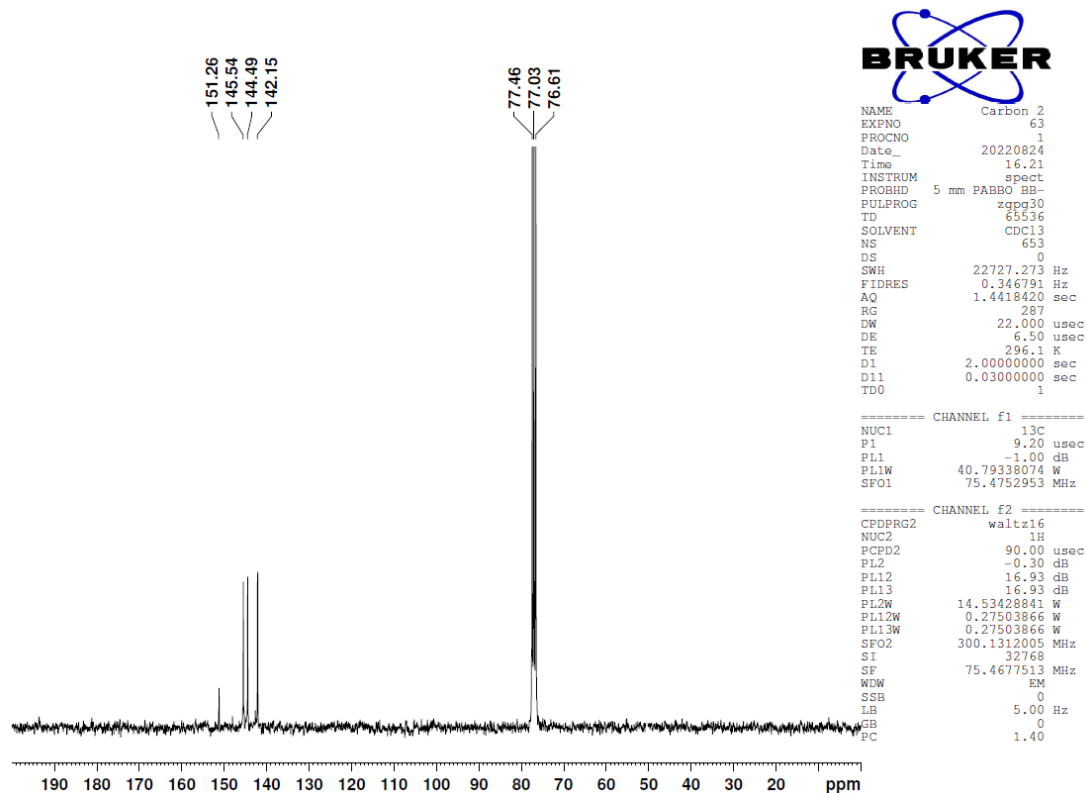


Fig S9: $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of bis(2-pyrazinyl)diselenide, $[(2\text{-pyzSe})_2]$ (2)

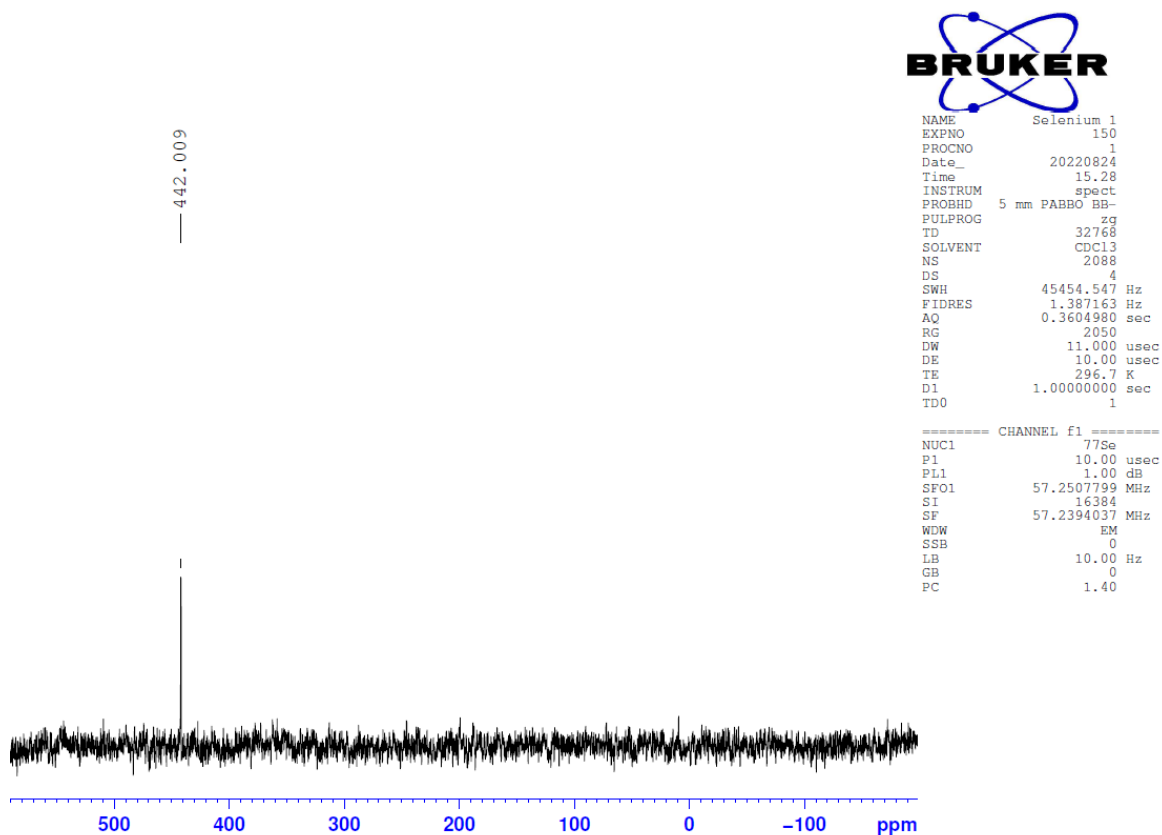


Fig S10: $^{77}\text{Se}\{^1\text{H}\}$ NMR spectra of bis(2-pyrazinyl)diselenide, $[(2\text{-pyzSe})_2]$ (2)

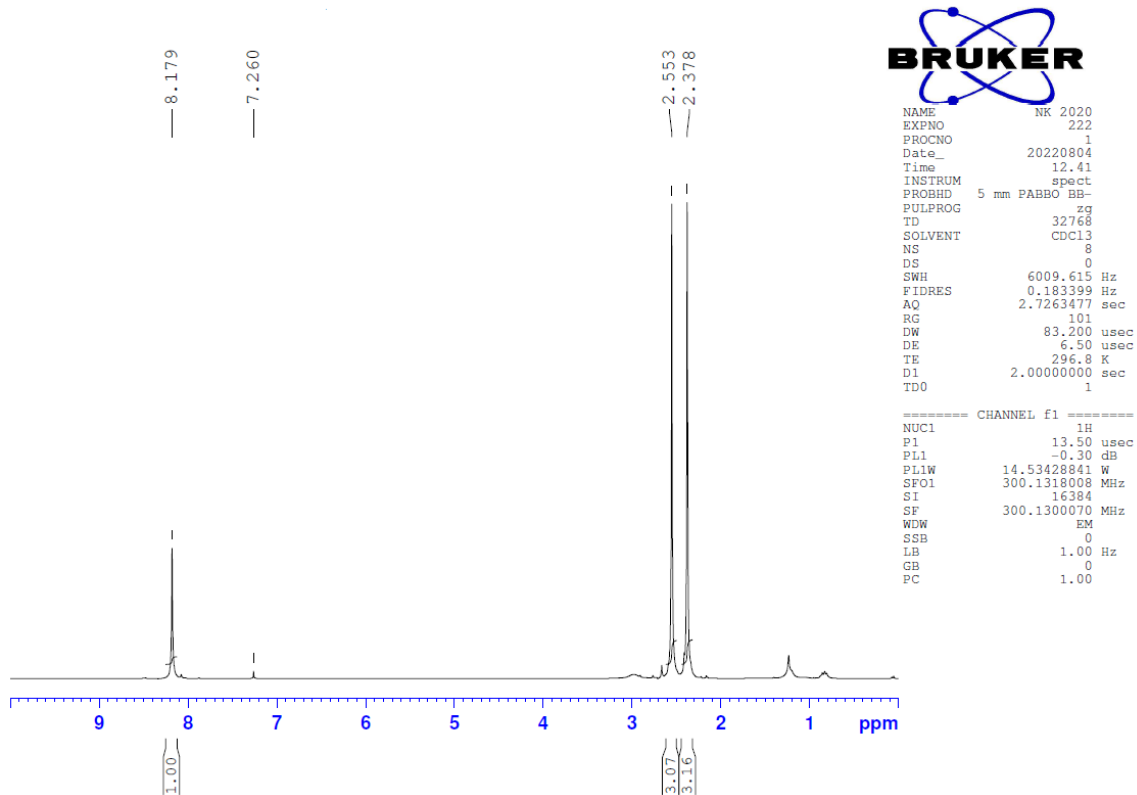


Fig S11: ^1H NMR spectra of bis(2,5-dimethyl-3-pyrazinyl)selenide, $[(2,5\text{-Me}_2\text{-3-pyz})_2\text{Se}]$ (3)

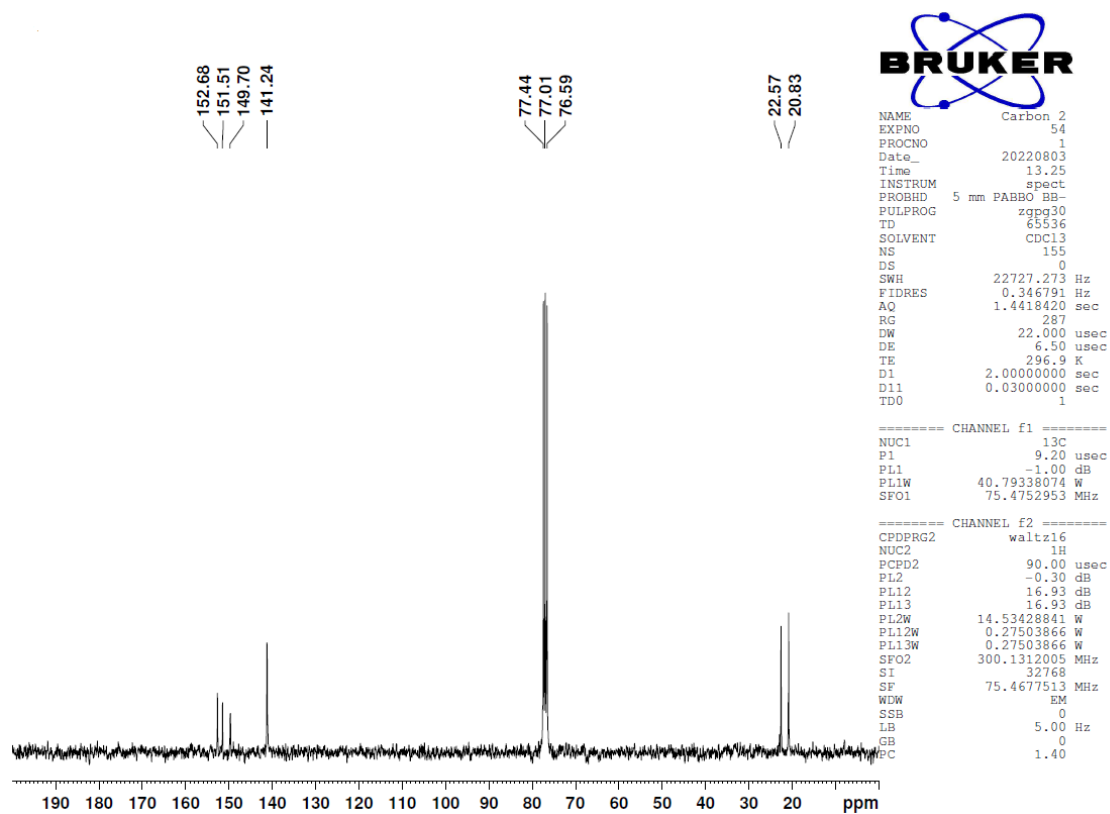


Fig S12: $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of Bis(2,5-dimethyl-3-pyrazinyl)selenide, $[(2,5\text{-Me}_2\text{-3-pyz})_2\text{Se}]$ (3)

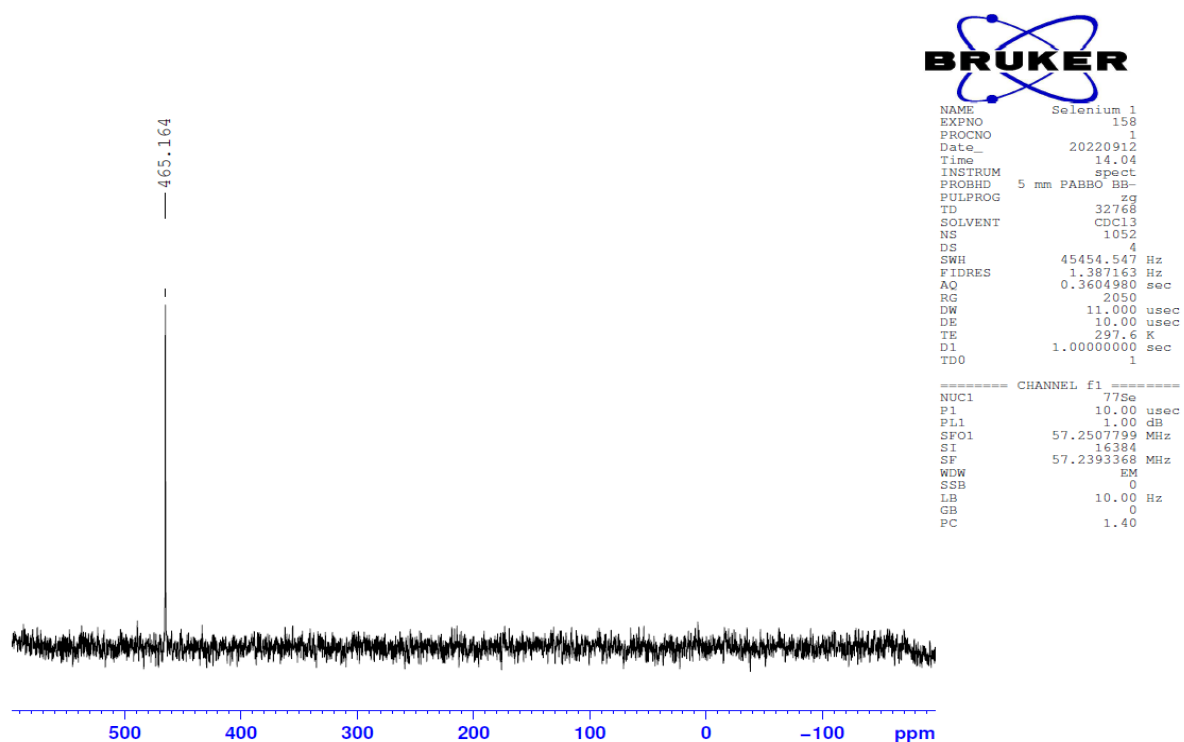


Fig S13: $^{77}\text{Se}\{^1\text{H}\}$ NMR spectra of Bis(2,5-dimethyl-3-pyrazinyl)selenide, [(2,5-Me₂-3-pyz)₂Se] (3).

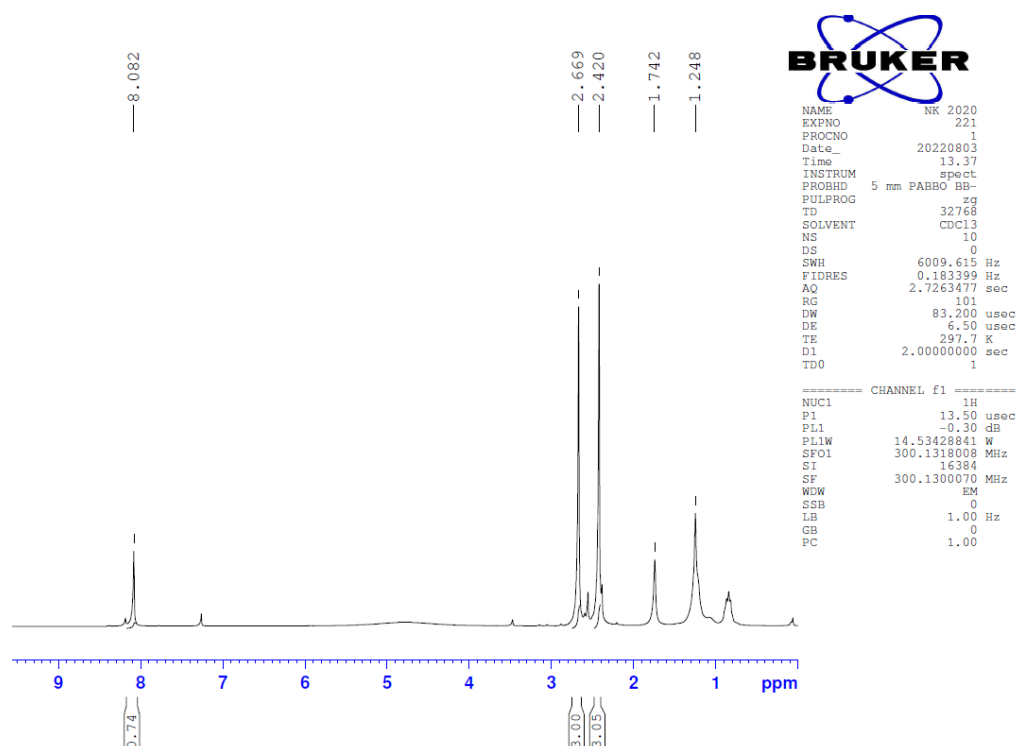


Fig S14: ^1H NMR spectra of Bis(2,5-dimethyl-3-pyrazinyl)diselenide, [(2,5-Me₂-3-pyzSe)₂] (4).

(Peaks at 1.24 and 1.74 is due to solvent residual signals) Ref: G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg *Organometallics* **29**(2010) 2176–2179.

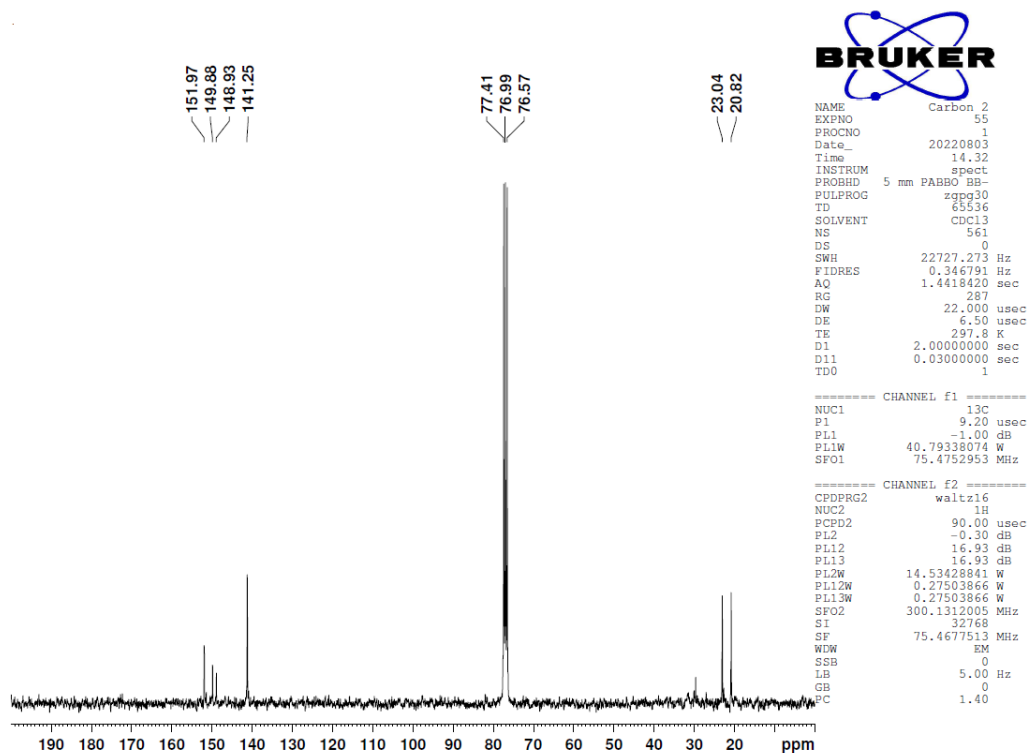


Fig S15: $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of Bis(2,5-dimethyl-3-pyrazinyl)diselenide [(2,5-Me₂-3-pyzSe)₂] (**4**)

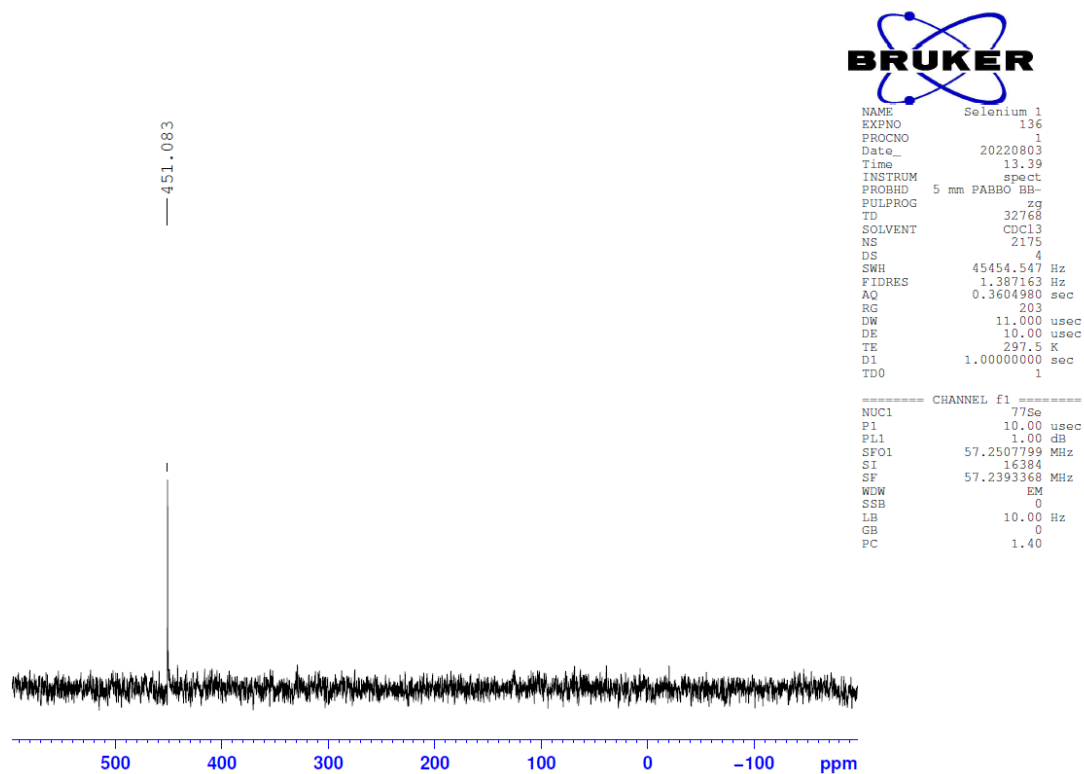


Fig S16: $^{77}\text{Se}\{^1\text{H}\}$ NMR spectra of Bis(2,5-dimethyl-3-pyrazinyl)diselenide [(2,5-Me₂-3-pyzSe)₂] (4)

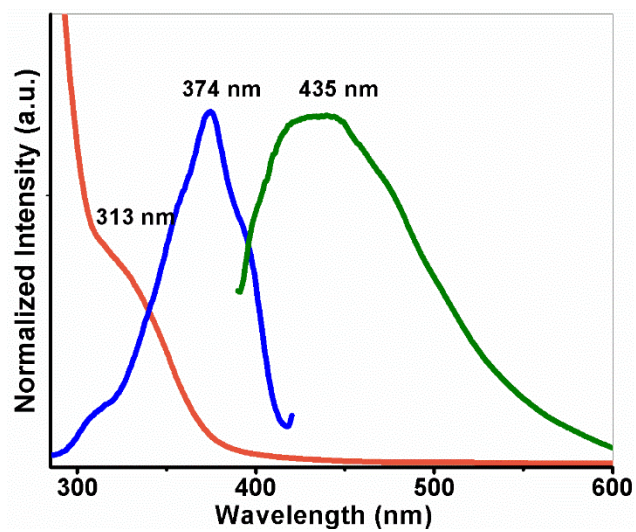


Fig S17: Absorption-, excitation-, emission-spectra of [(3-Me-2-pySe)₂].

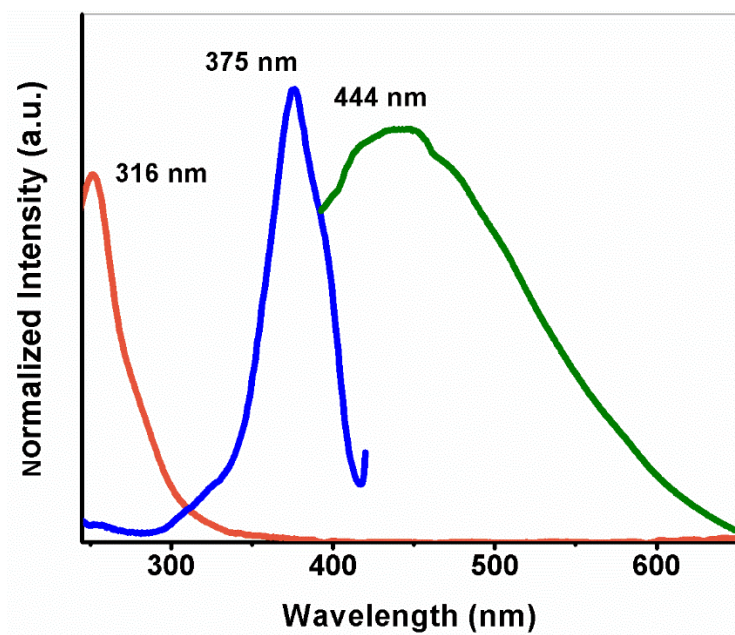


Fig S18: Absorption-, excitation-, emission-spectra of [(4,6-Me₂-2-pymSe)₂].