

Supplementary Information

Structure/Activity of Pt^{II}/*N,N*-Disubstituted-*N'*-acylthiourea Complexes: Anti-Tumor and Anti-*Mycobacterium tuberculosis* Activities

Ana M. Plutín,^{*a} Anislay Alvarez,^a Raúl Mocoelo,^a Raúl Ramos,^a Osmar C. Sánchez,^a
Eduardo E. Castellano,^b Monize M. da Silva,^c Wilmer Villarreal,^c Legna Colina-Vegas,^c
Fernando R. Pavan^d and Alzir A. Batista^{*c}

^aLaboratorio de Síntesis Orgánica, Facultad de Química, Universidad de La Habana, 10400 La Habana, Cuba

^bInstituto de Física de São Carlos, Universidade de São Paulo, 05508-090 São Carlos-SP, Brazil

^cDepartamento de Química, Universidade Federal de São Carlos, 13565-905 São Carlos-SP, Brazil

^dFaculdade de Ciências Farmacêuticas, Universidade Estadual Paulista (UNESP), 14800-903 Araraquara-SP, Brazil

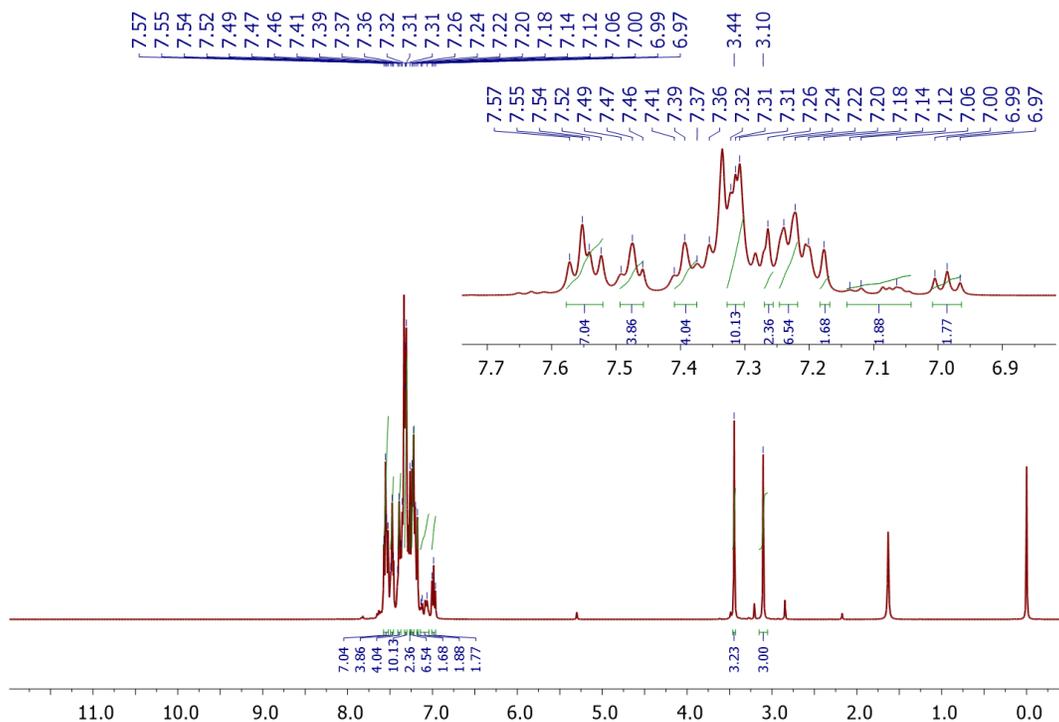


Figure S1. ¹H NMR (400 MHz, CDCl₃) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-dimethyl-*N'*-benzoylthioureaato-*k*²O,*S*)]PF₆ (1).

*e-mail: anap@fq.uh.cu; daab@ufscar.br

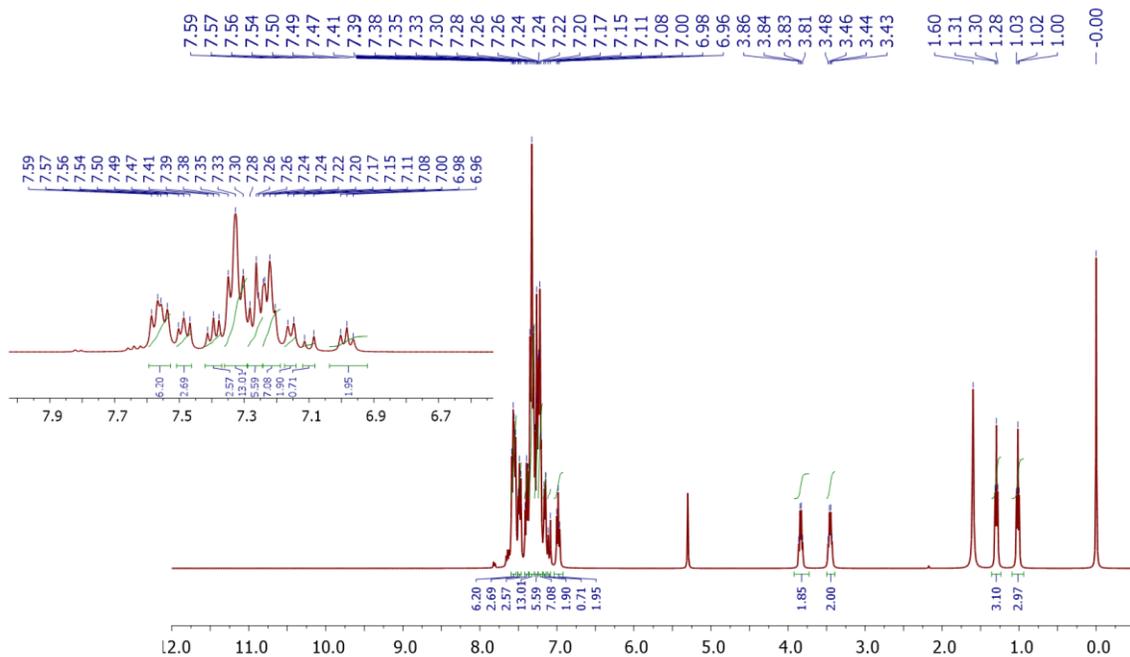


Figure S2. ^1H NMR (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-diethyl-*N'*-benzoylthioureato-*k*²O,*S*)]PF₆ (**2**).

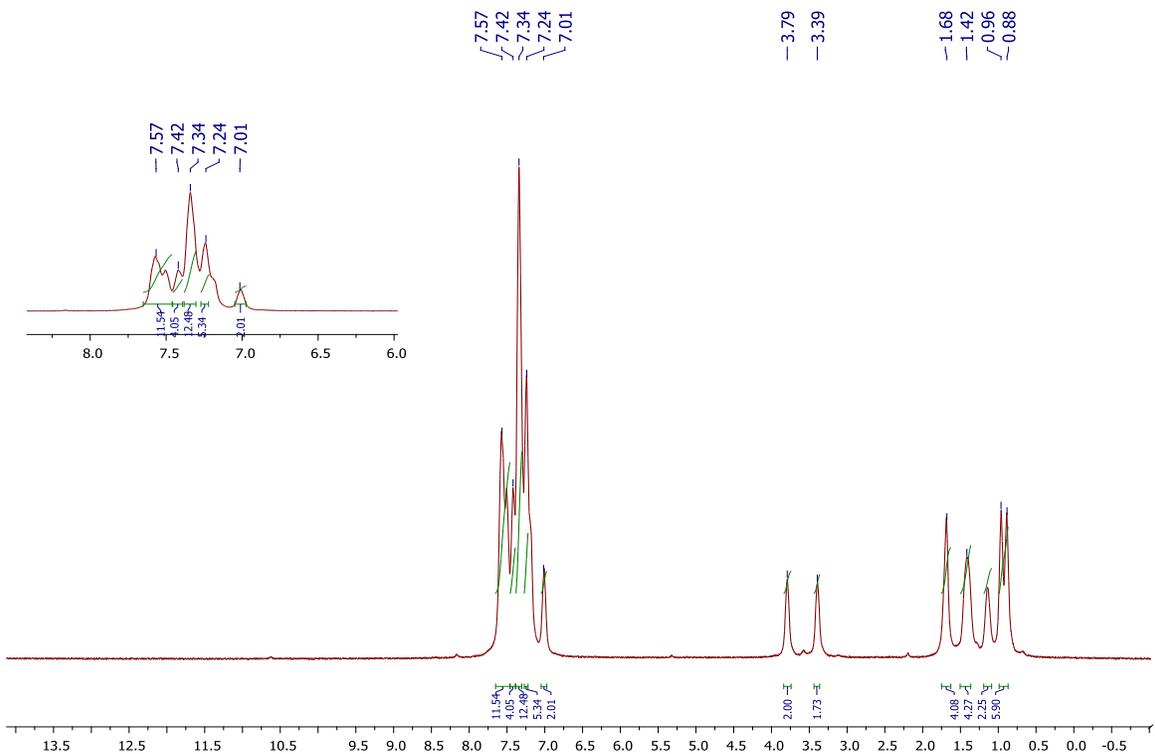


Figure S3. ^1H NMR (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-dibutyl-*N'*-benzoylthioureato-*k*²O,*S*)]PF₆ (**3**).

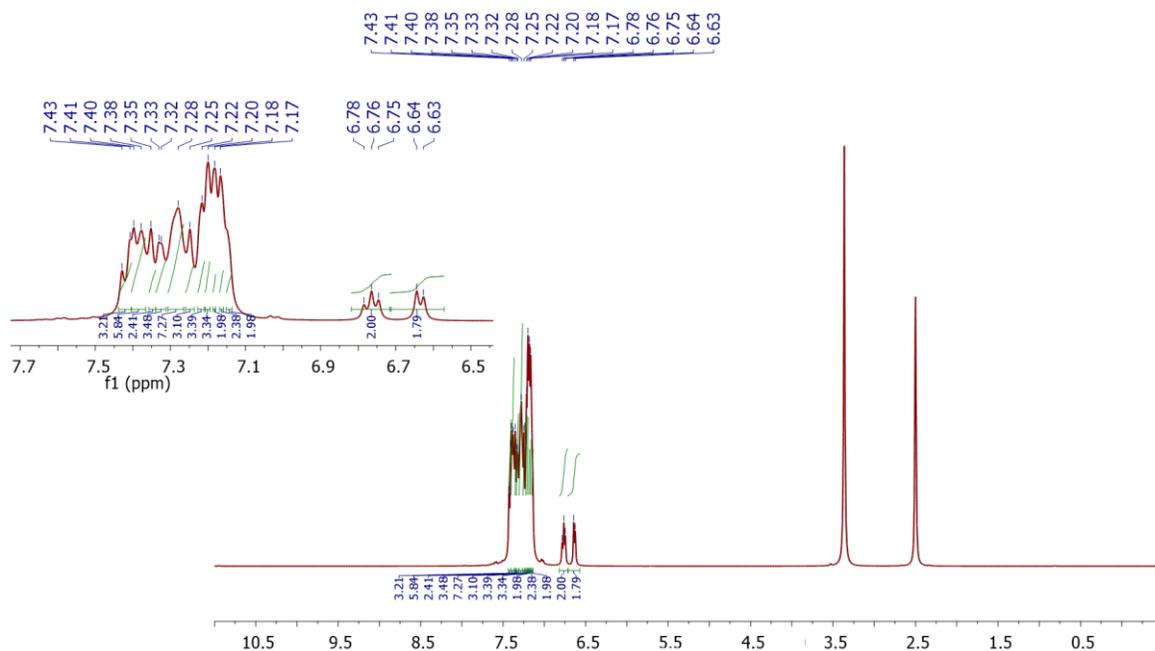


Figure S4. ^1H NMR (400 MHz, CDCl_3 , drops DMSO) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-diphenyl-*N'*-benzoylthioureato- $k^2\text{O,S}$)]PF₆ (**4**).

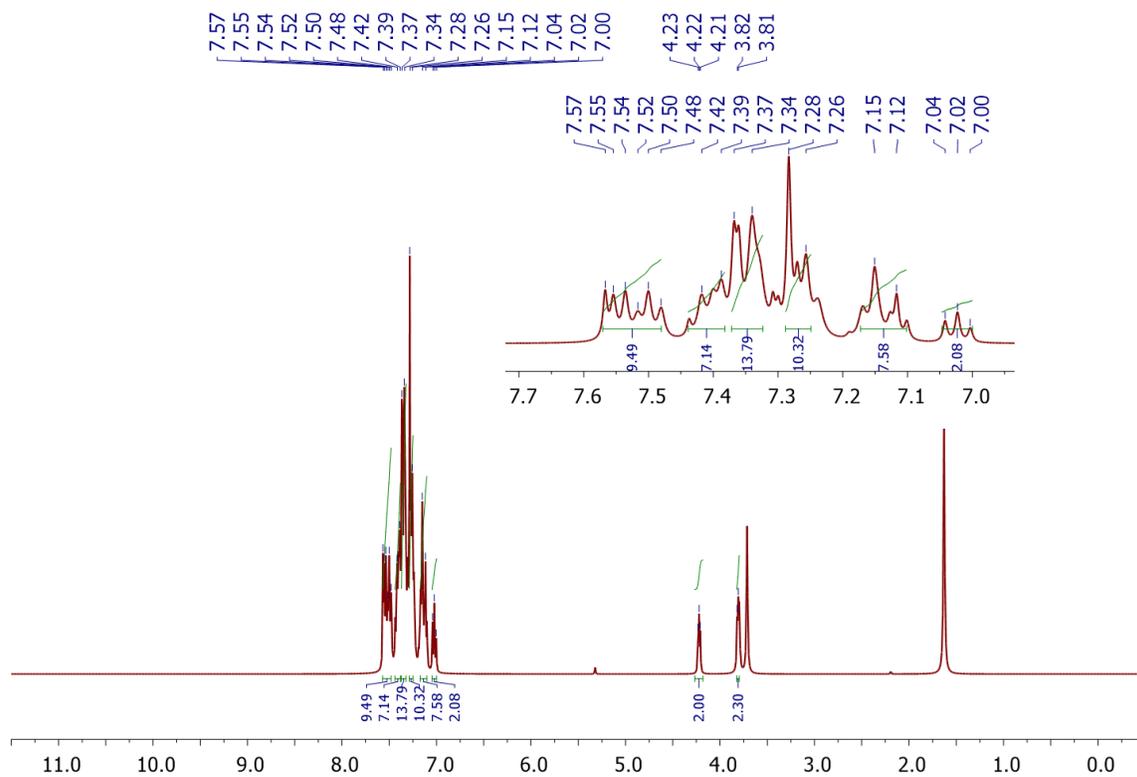


Figure S5. ^1H NMR (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-dibenzyl-*N'*-benzoylthioureato- $k^2\text{O,S}$)]PF₆ (**5**).

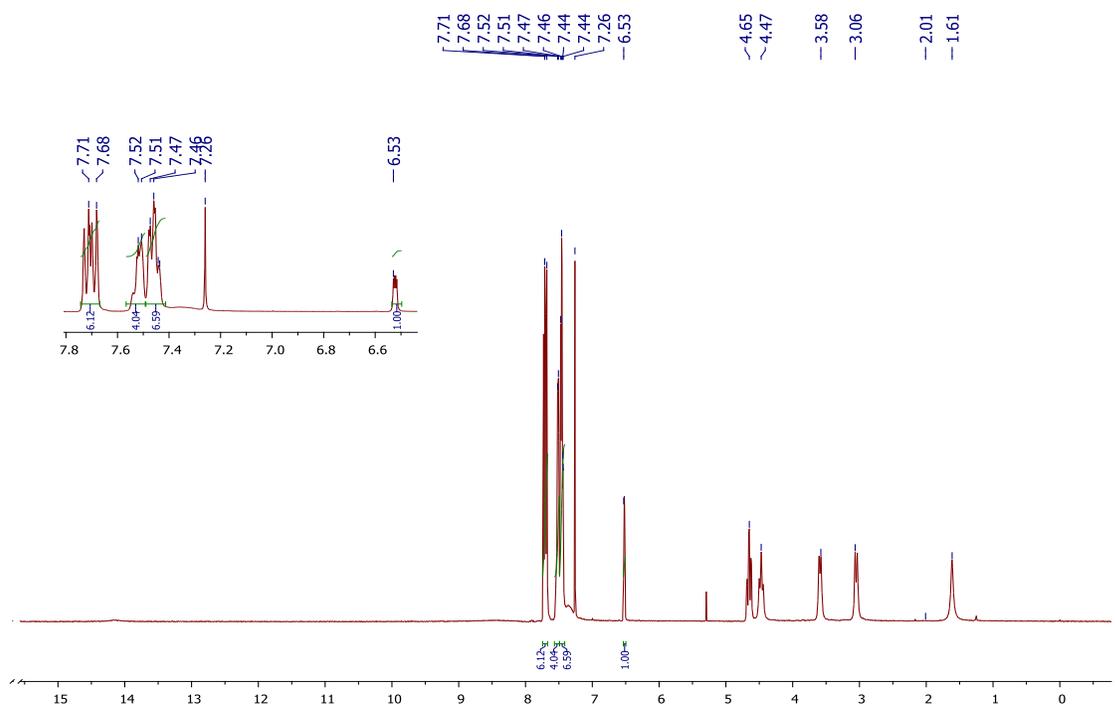


Figure S6. ^1H NMR (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-diethyl-*N'*-furoylthioureato-*k*²O,*S*)]PF₆ (**6**).

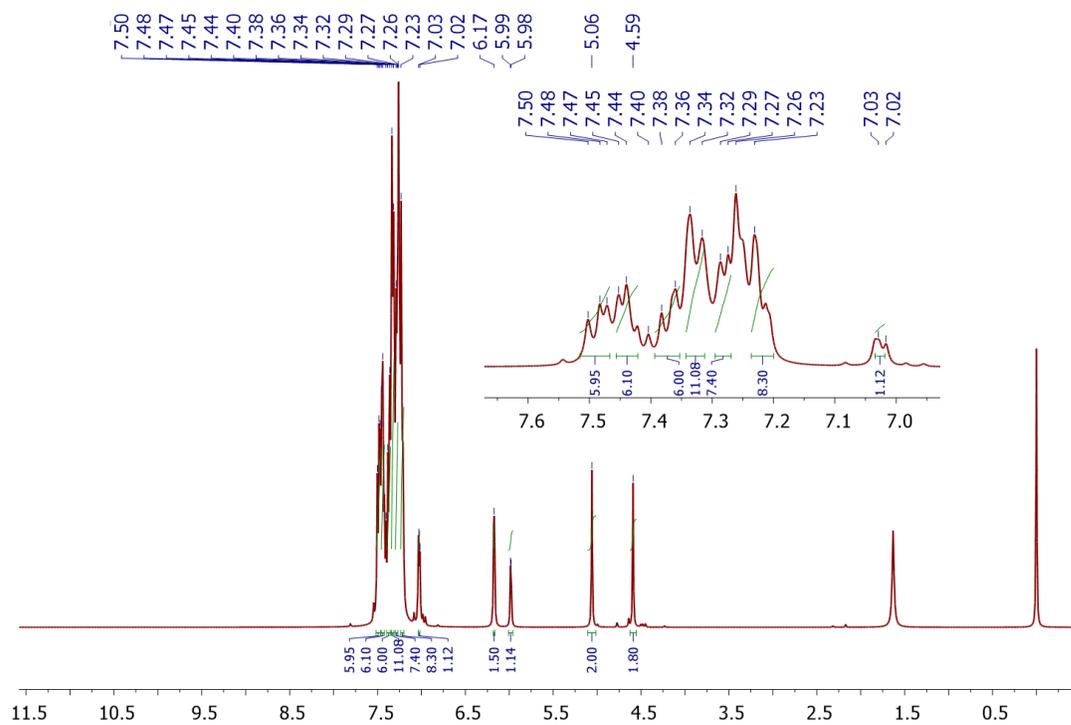


Figure S7. ^1H NMR (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-dibenzyl-*N'*-furoylthioureato-*k*²O,*S*)]PF₆ (**7**).

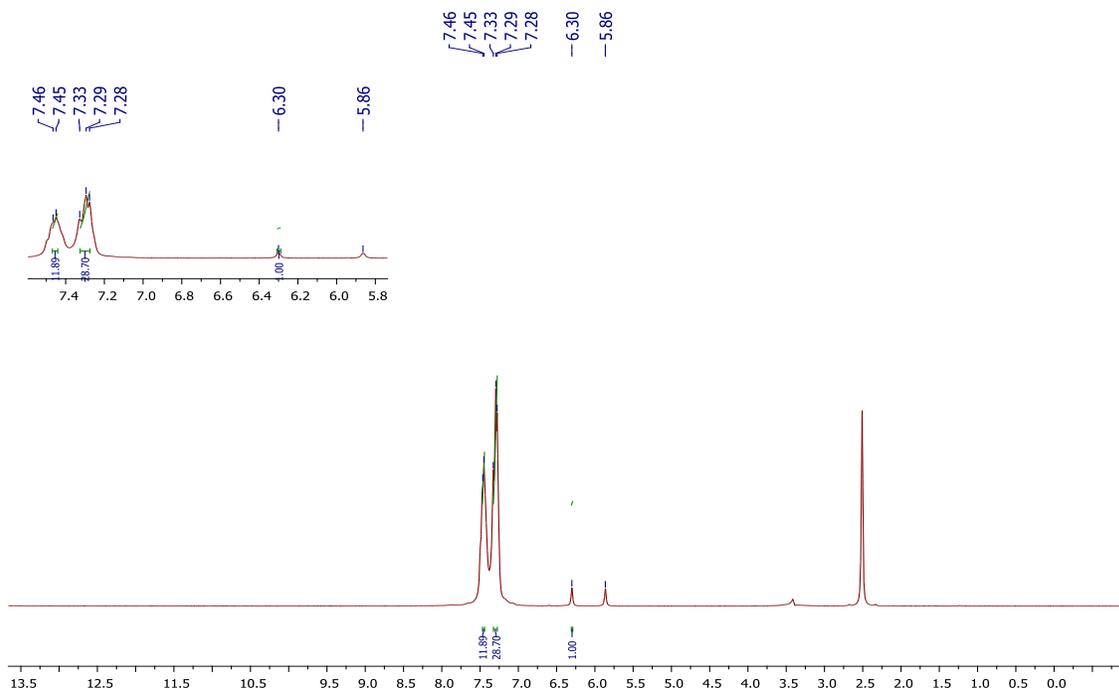


Figure S8. ^1H NMR (400 MHz, DMSO) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-diphenyl-*N'*-furoylthioureato-*k*²O,*S*)]PF₆ (**8**).

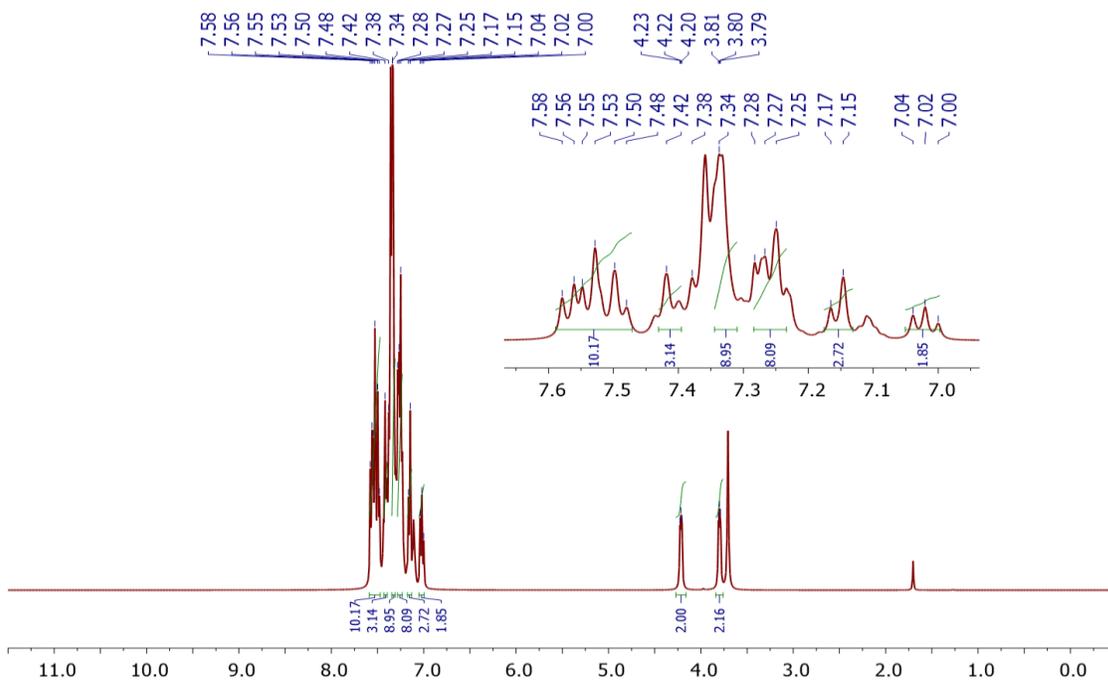


Figure S9. ^1H NMR (400 MHz, CDCl₃) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-morpholine-*N'*-furoylthioureato-*k*²O,*S*)]PF₆ (**9**).

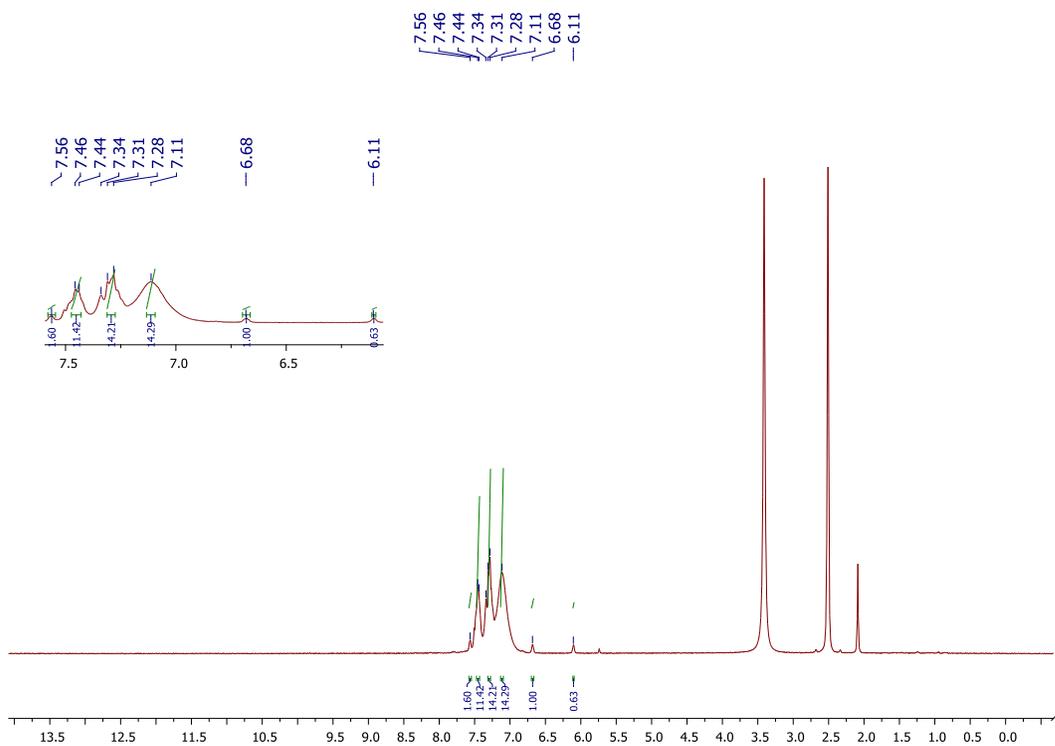


Figure S10. ^1H NMR (400 MHz, DMSO) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-diphenyl-*N'*-thiophenylthioureato-*k*²O,*S*)]PF₆ (**11**).

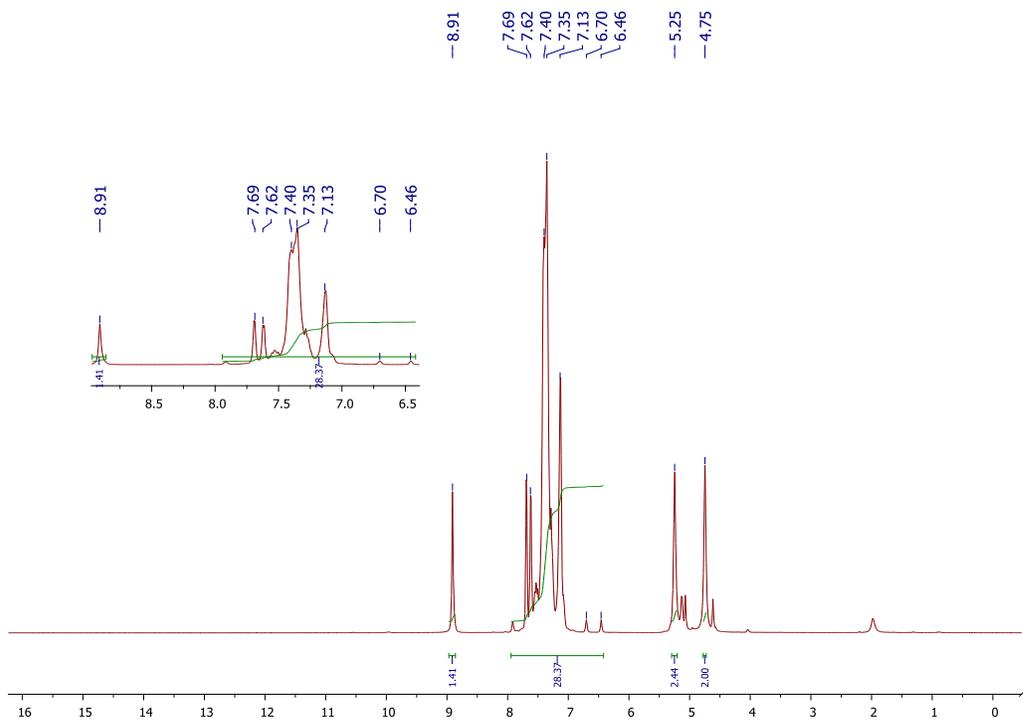


Figure S11. ^1H NMR (400 MHz, CDCl₃) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-dibenzyl-*N'*-thiophenylthioureato-*k*²O,*S*)]PF₆ (**12**).

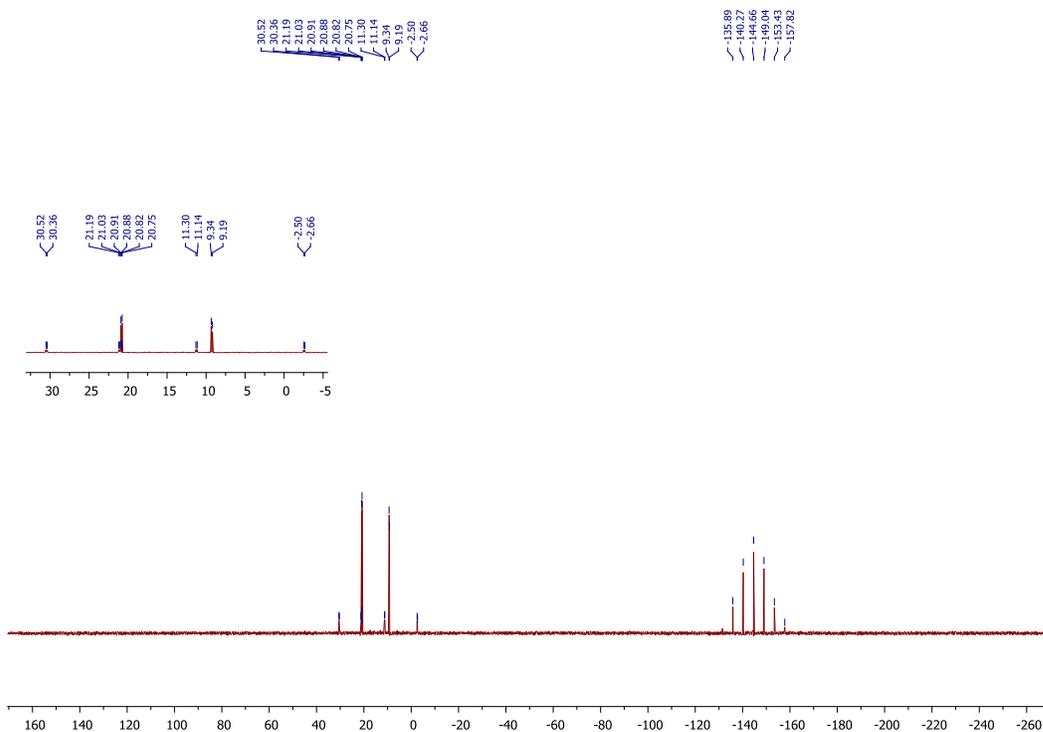


Figure S12. $^{31}\text{P}\{^1\text{H}\}$ (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-dimethyl-*N'*-benzoylthioureato-*k*²O,*S*)]PF₆ (**1**).

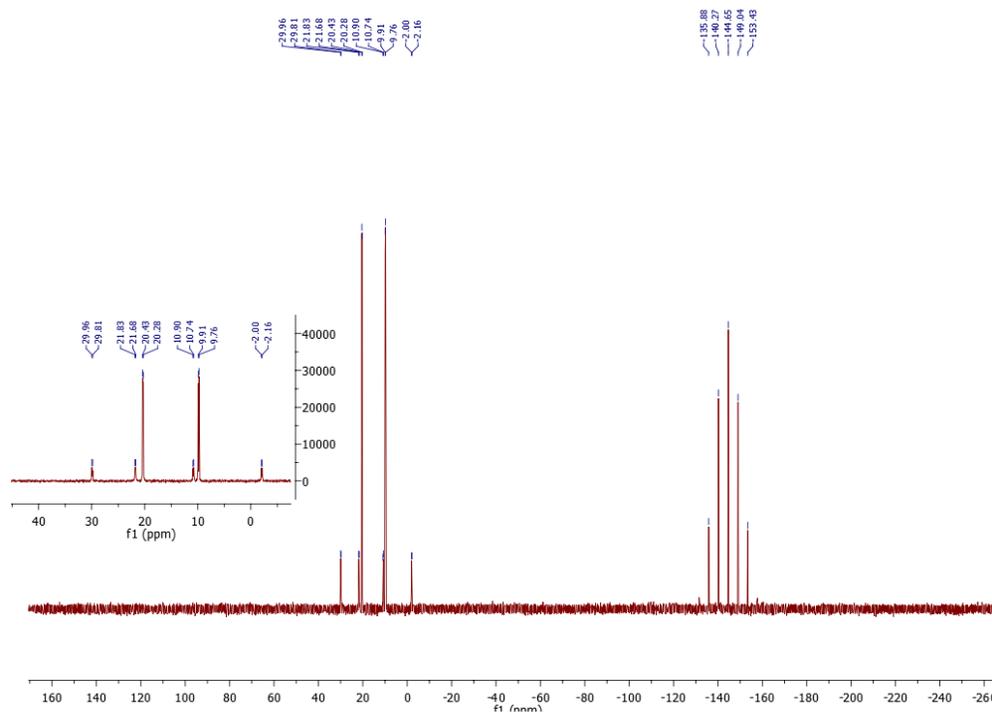


Figure S13. $^{31}\text{P}\{^1\text{H}\}$ (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-diethyl-*N'*-benzoylthioureato-*k*²O,*S*)]PF₆ (**2**).

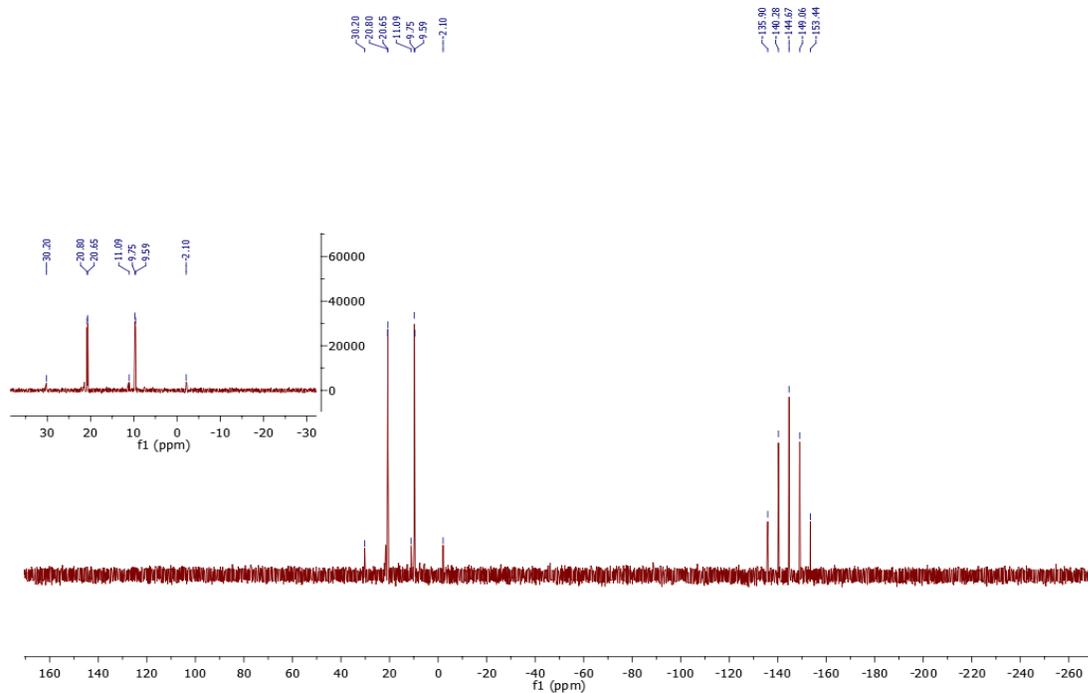


Figure S14. $^{31}\text{P}\{^1\text{H}\}$ (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-dibutyl-*N'*-benzoylthioureato-*k*²O,*S*)]PF₆ (**3**).

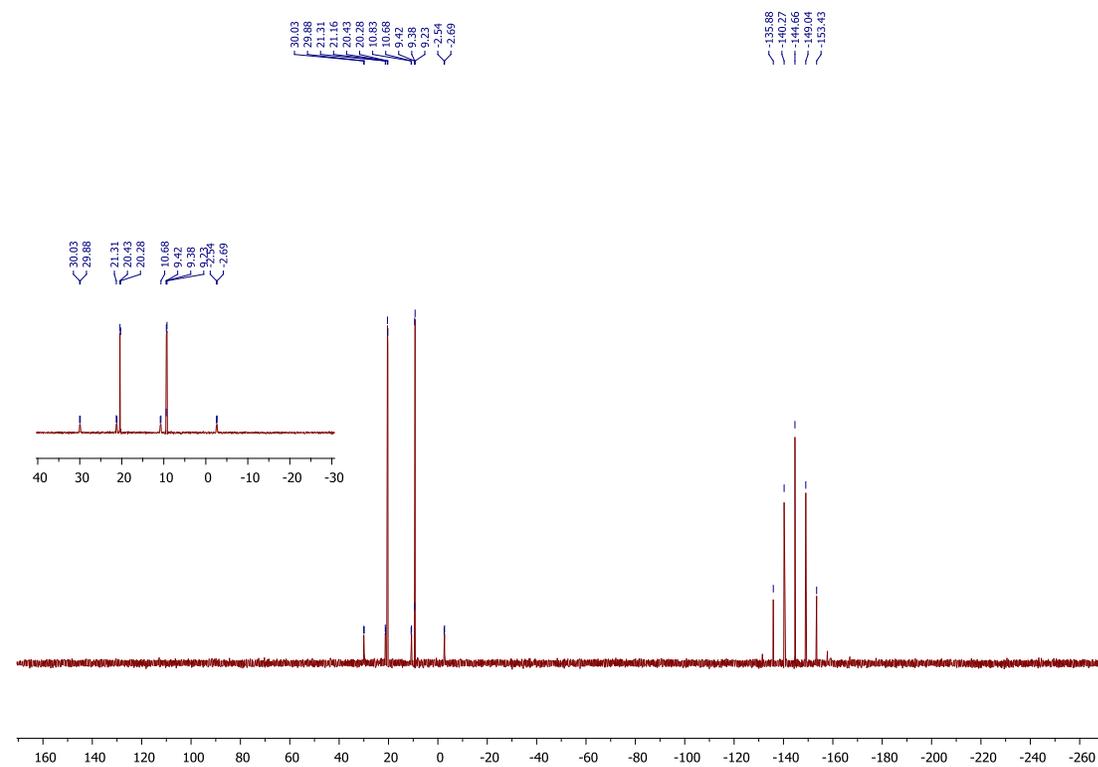


Figure S15. $^{31}\text{P}\{^1\text{H}\}$ (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-diphenyl-*N'*-benzoylthioureato-*k*²O,*S*)]PF₆ (**4**).

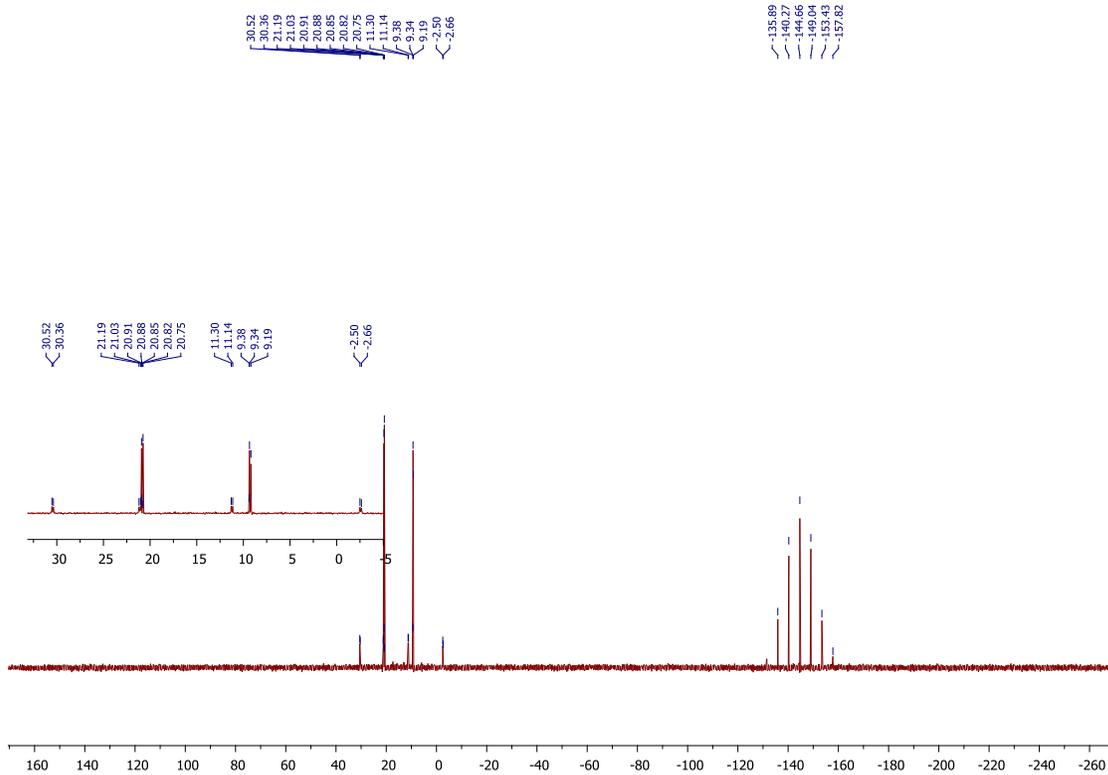


Figure S16. $^{31}\text{P}\{^1\text{H}\}$ (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-dibenzyl-*N'*-benzoylthioureato- $\text{k}^2\text{O,S}$)]PF₆ (**5**).

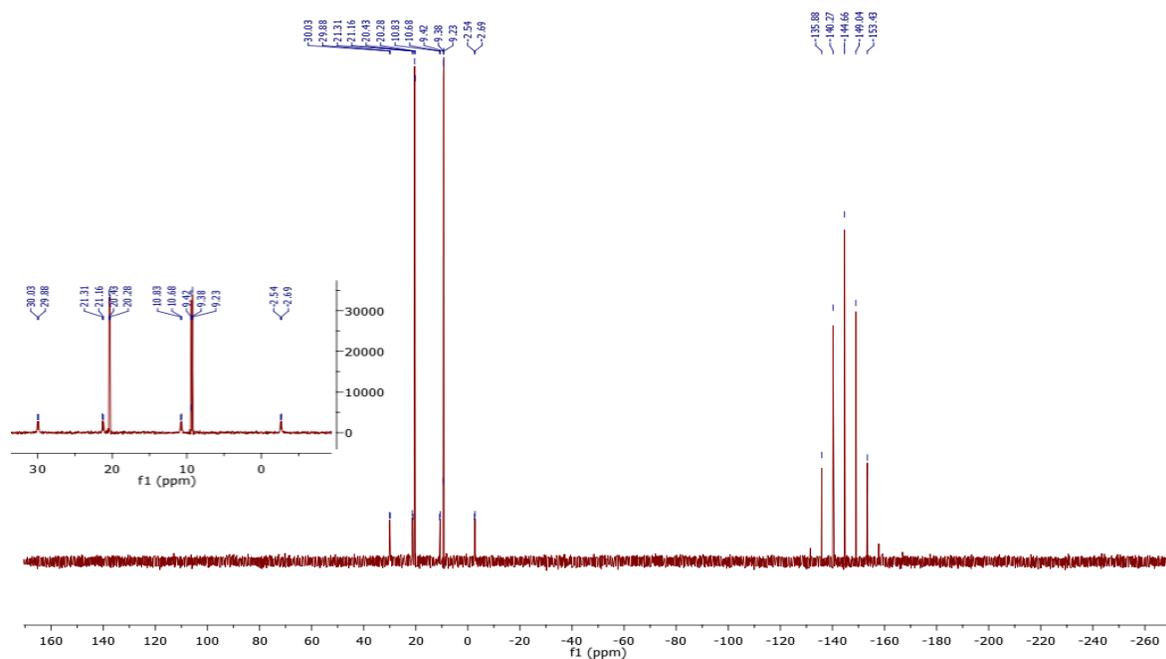


Figure S17. $^{31}\text{P}\{^1\text{H}\}$ (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-diethyl-*N'*-furoylthioureato- $\text{k}^2\text{O,S}$)]PF₆ (**6**).

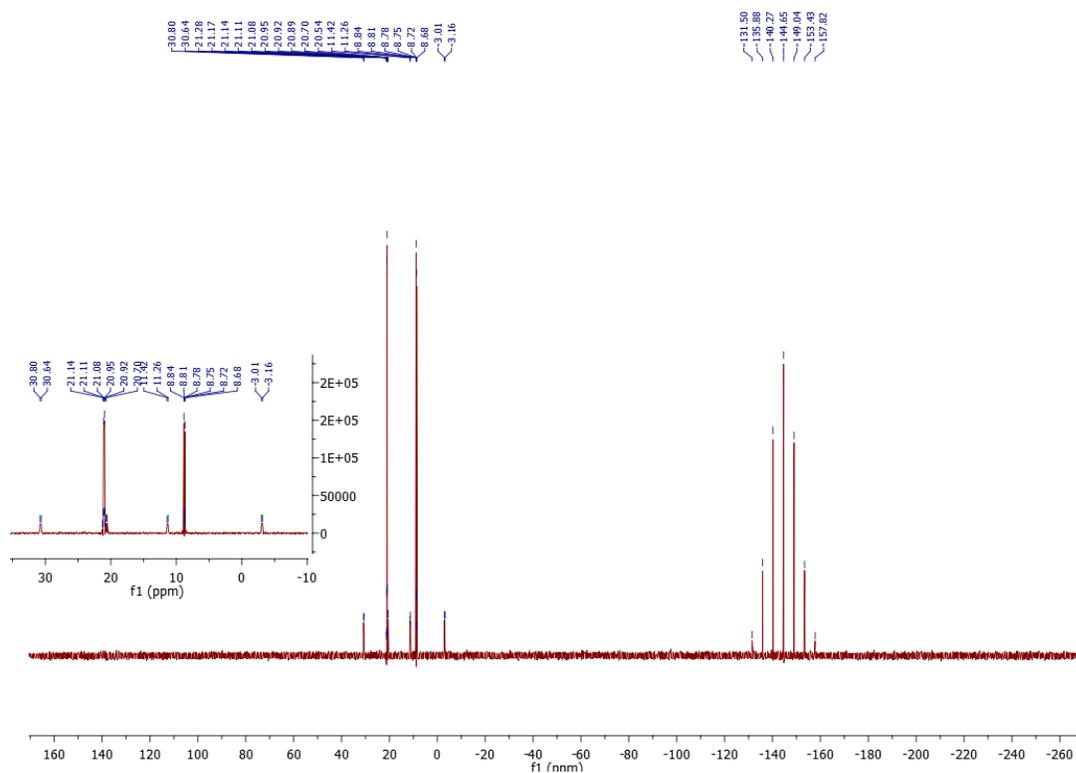


Figure S20. $^{31}\text{P}\{^1\text{H}\}$ (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-morpholine-*N'*-furoylthioureato-*k*²O,*S*)]PF₆ (**9**).

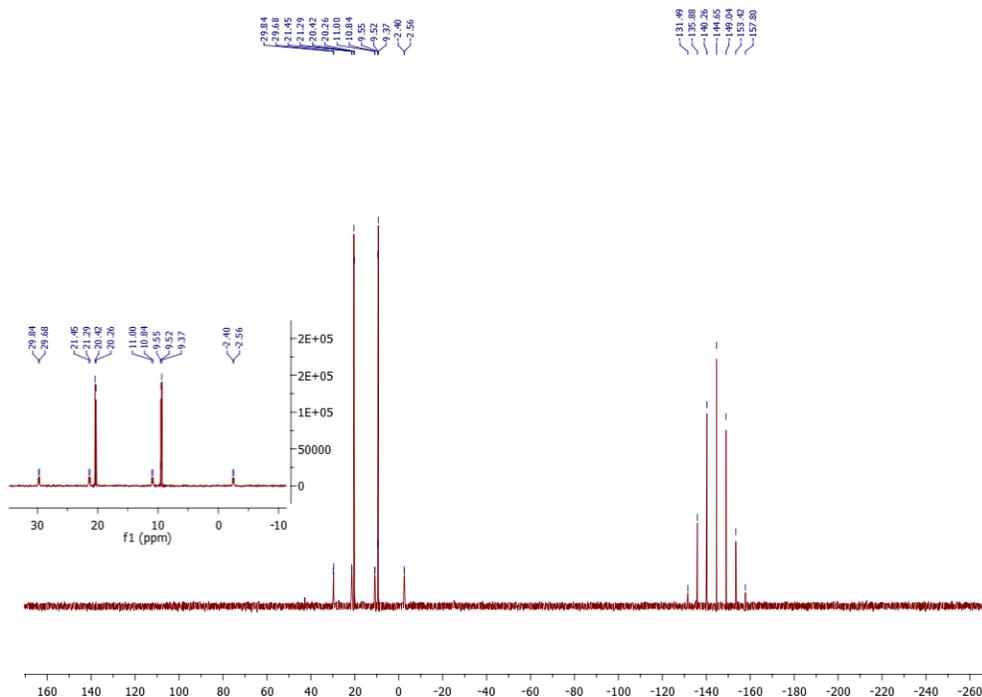


Figure S21. $^{31}\text{P}\{^1\text{H}\}$ (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(*N,N*-diphenyl-*N'*-thiophenylthioureato-*k*²O,*S*)]PF₆ (**11**).

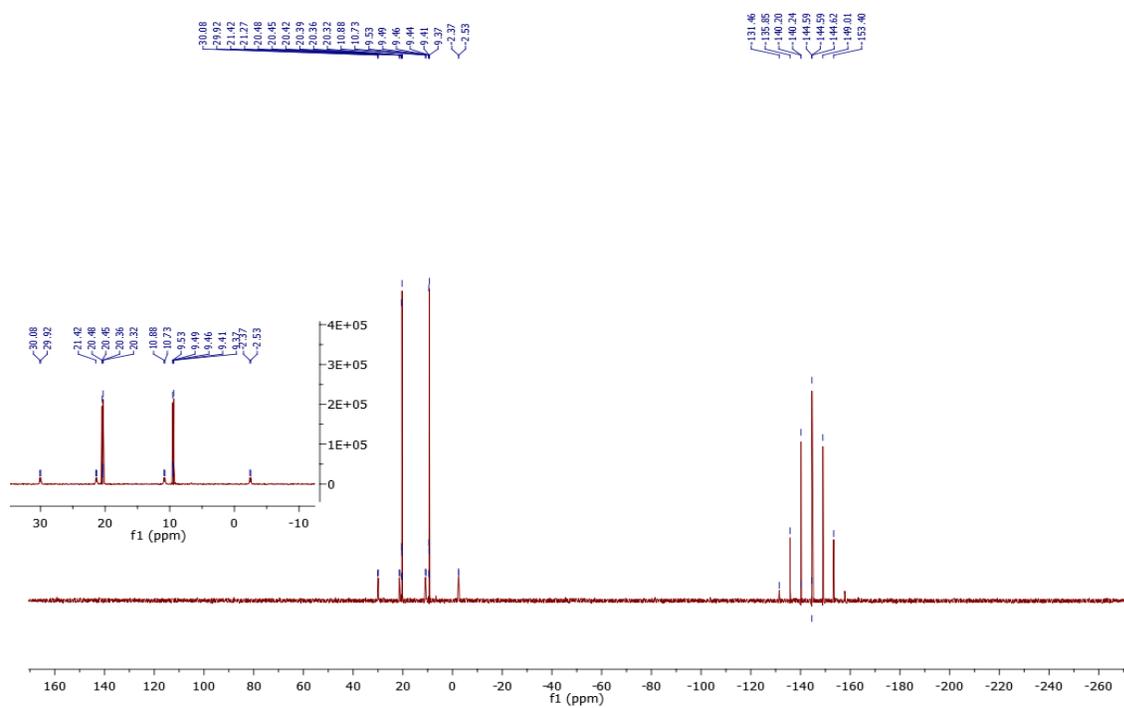


Figure S22. $^{31}\text{P}\{^1\text{H}\}$ (400 MHz, CDCl_3) spectrum of *cis*-[Pt(PPh₃)₂(N,N-dibenzyl-N'-thiophenylthioureato-k²O,S)]PF₆ (**12**).