Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Exploring structure relationships and mitochondrial activity of *fac*-$\{M^{I}(CO)_3\}^+$ bis(diarylphosphino)alkyl-/arylamine complexes (M=^{99}Tc, Re)

Dumisani V. Kama,[a] Angelo Frei,[b] Marietjie Schutte-Smith,[a] Alice Brink,[a] Chantel Swart,[c] Henrik Braband,[b] Roger Alberto[b,] and Andreas Roodt[a,]**

[a]Department of Chemistry, University of the Free State, PO Box 339, Bloemfontein, 9300;
[b]Depatment of Chemistry, University of Zürich, Winterthurerstrasse 190, 8057 Zürich, Switzerland.
[c]Department of Biochemistry, University of the Free State, PO Box 339, Bloemfontein, 9300.

Table of Contents

Figure S1 ^{1}H NMR spectrum for *fac*-[Re(Cy-pTolPNP)(CO)$_3$Br] (**1A**)

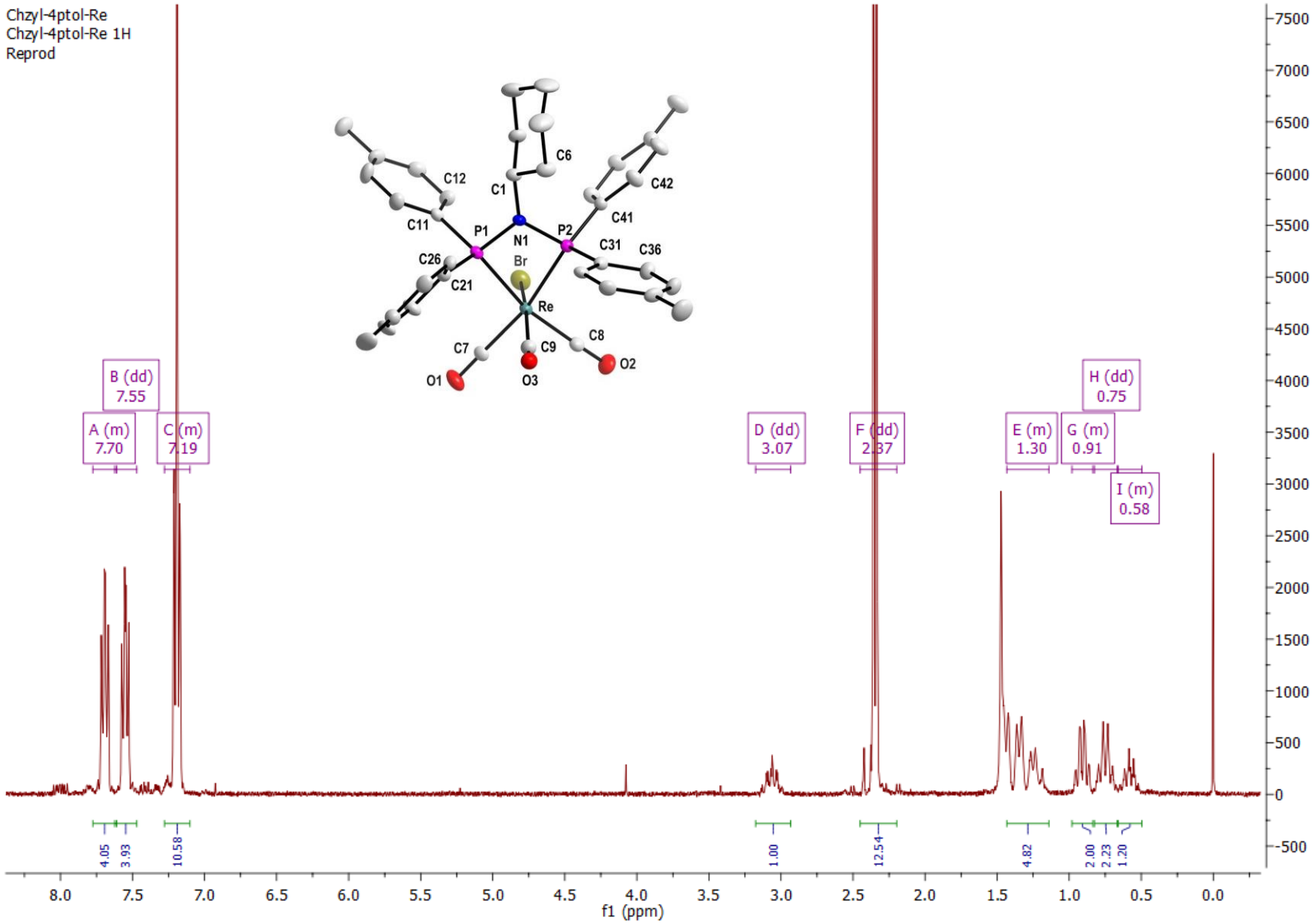

Figure S2 ^{31}P NMR spectrum for *fac*-[Re(Cy-pTolPNP)(CO)$_3$Br] (**1A**)

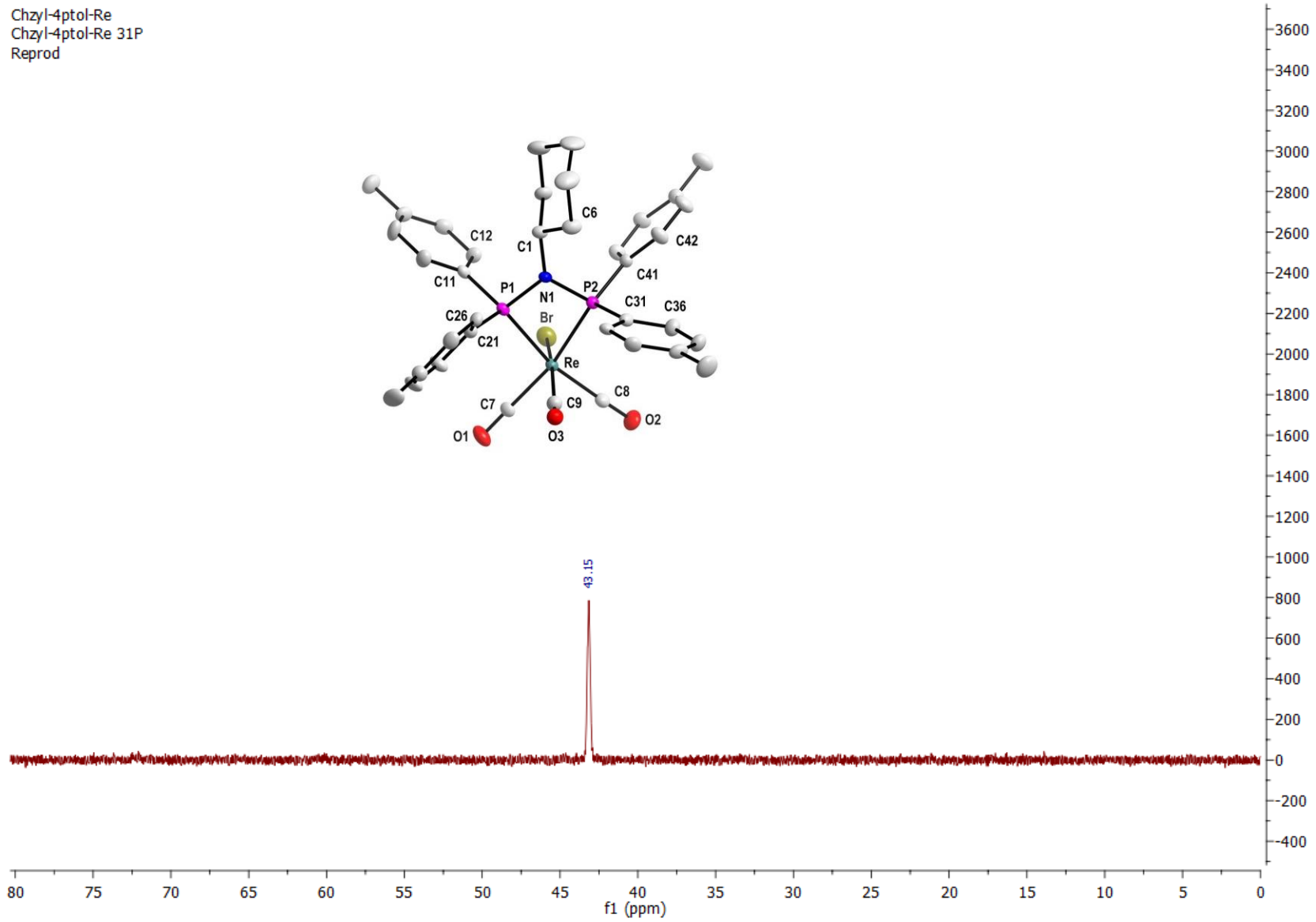

Figure S3 IR spectrum for *fac*-[Re(Cy-pTolPNP)(CO)$_3$Br] (**1A**) ATR

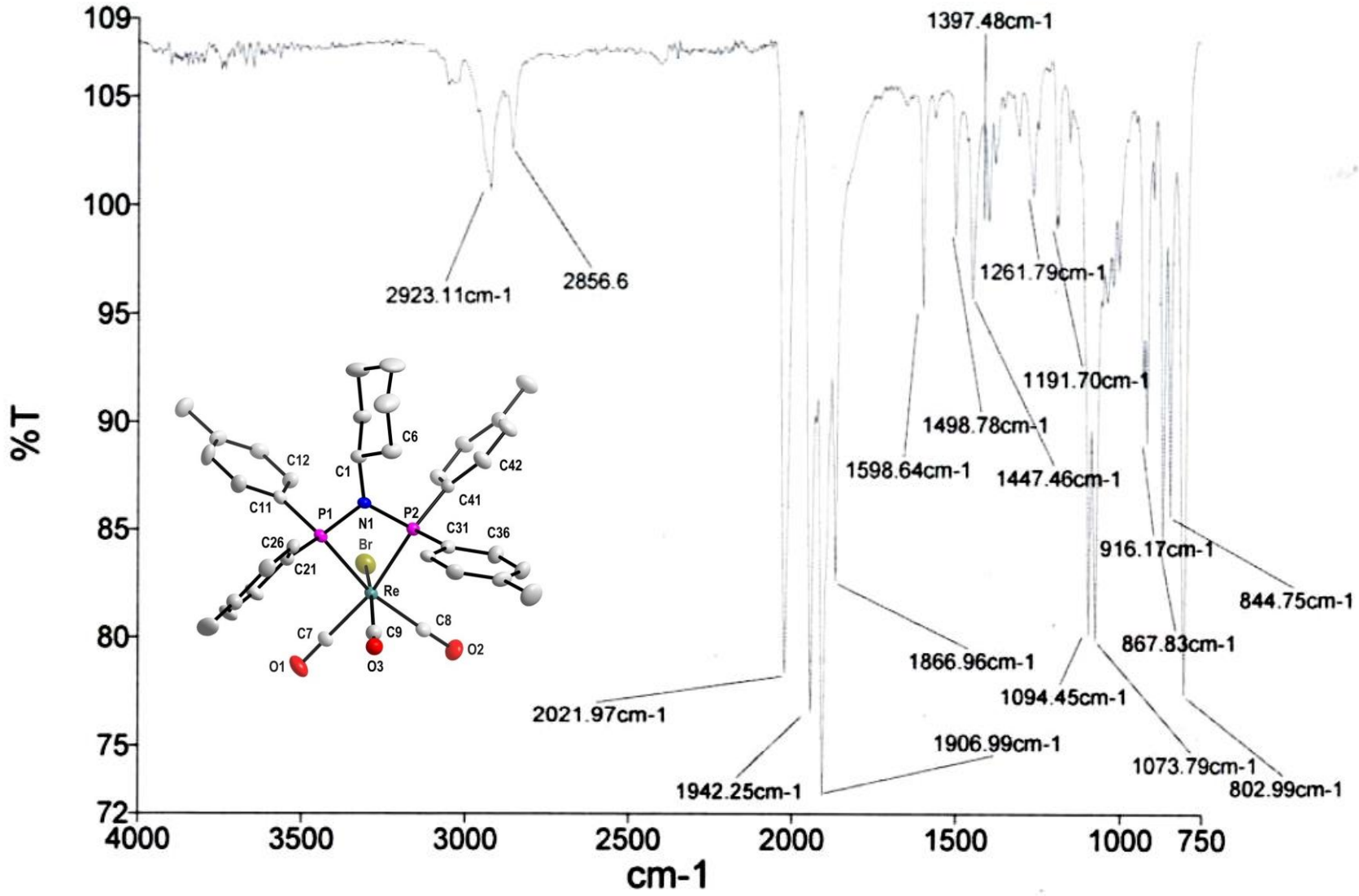

Figure S4 IR spectrum for *fac*-[Re(Cy-pTolPNP)(CO)$_3$Br] (**1A**) DCM

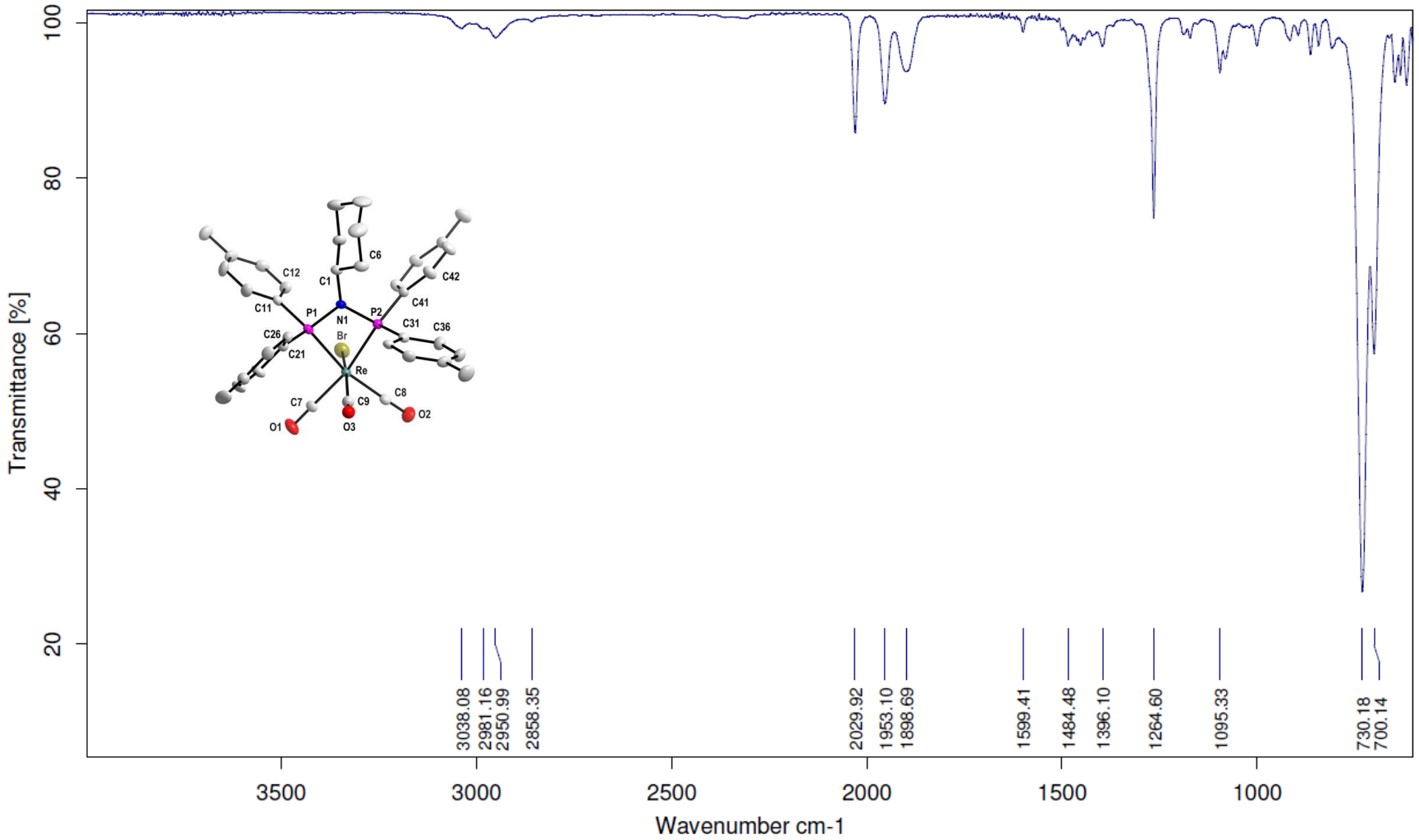

Figure S5 Disordered *fac*-[Re(Cy-pTolPNP)(CO)3Br] (**1A**); Illustrated by Br1B.

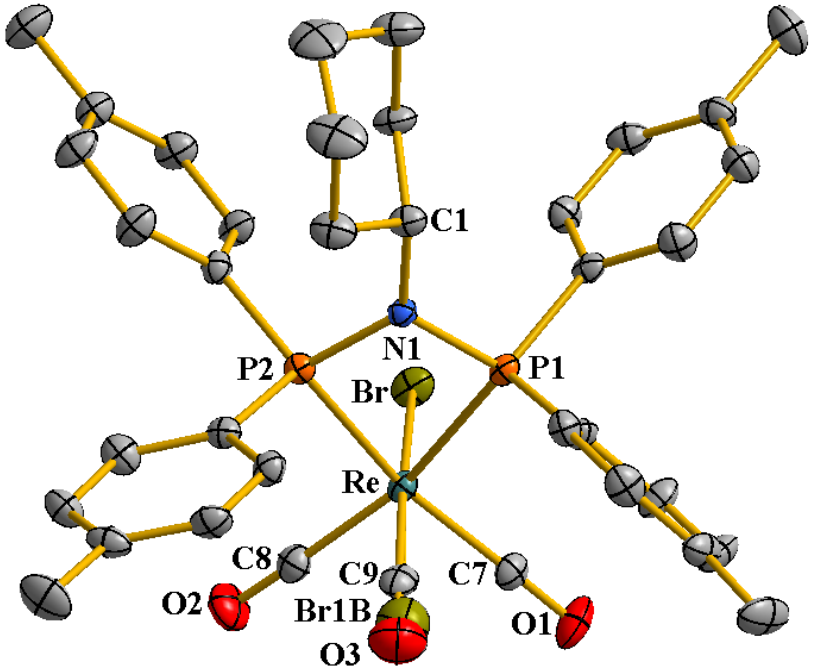

Figure S6 ^{1}H NMR spectrum for *fac*-[^{99}Tc(Cy-*p*TolPNP)(CO)$_3$Cl] (**1B**)

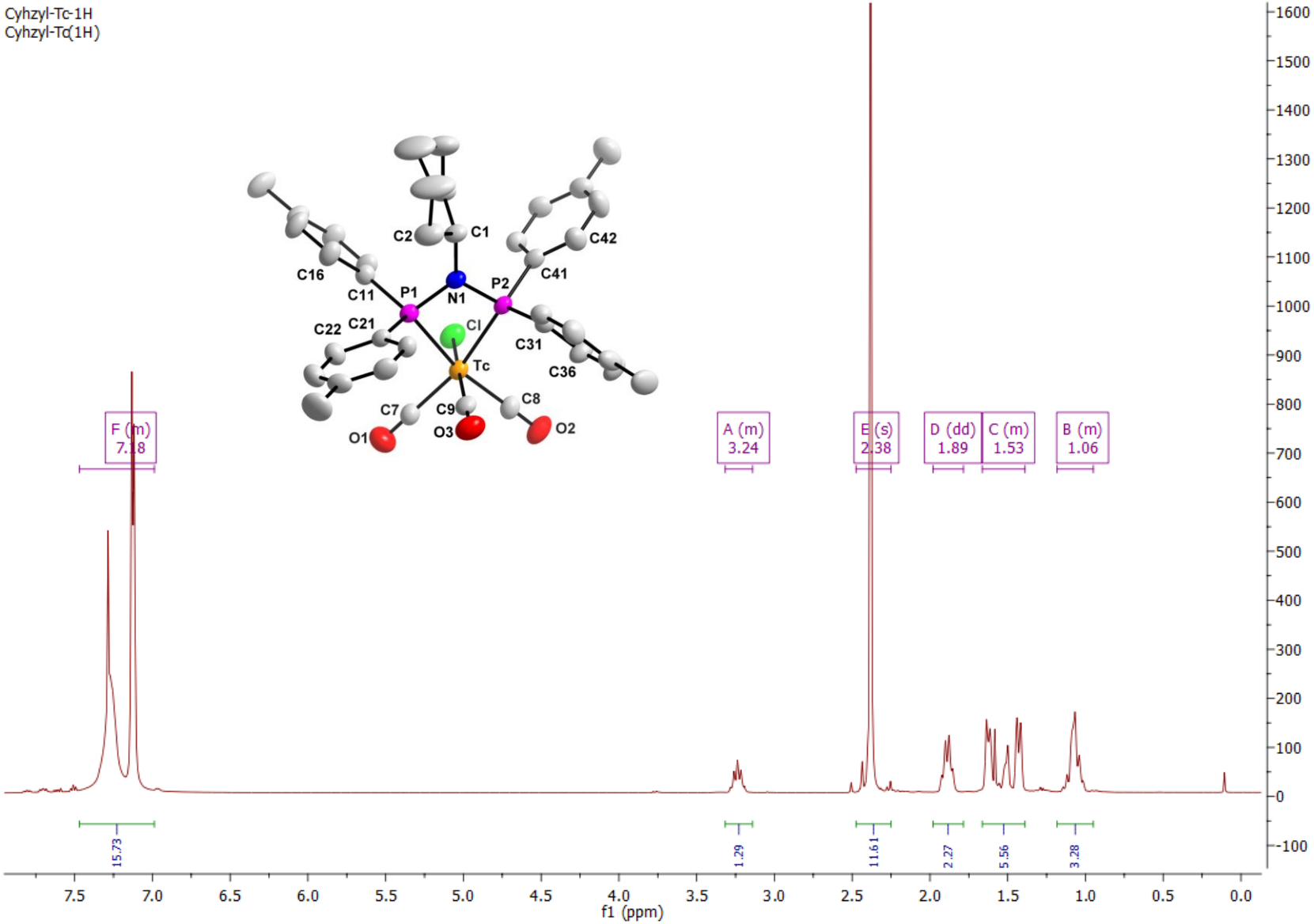

Figure S7 ^{99}Tc NMR spectrum for *fac*-[^{99}Tc(Cy-*p*TolPNP)(CO)$_3$Cl] (**1B**)

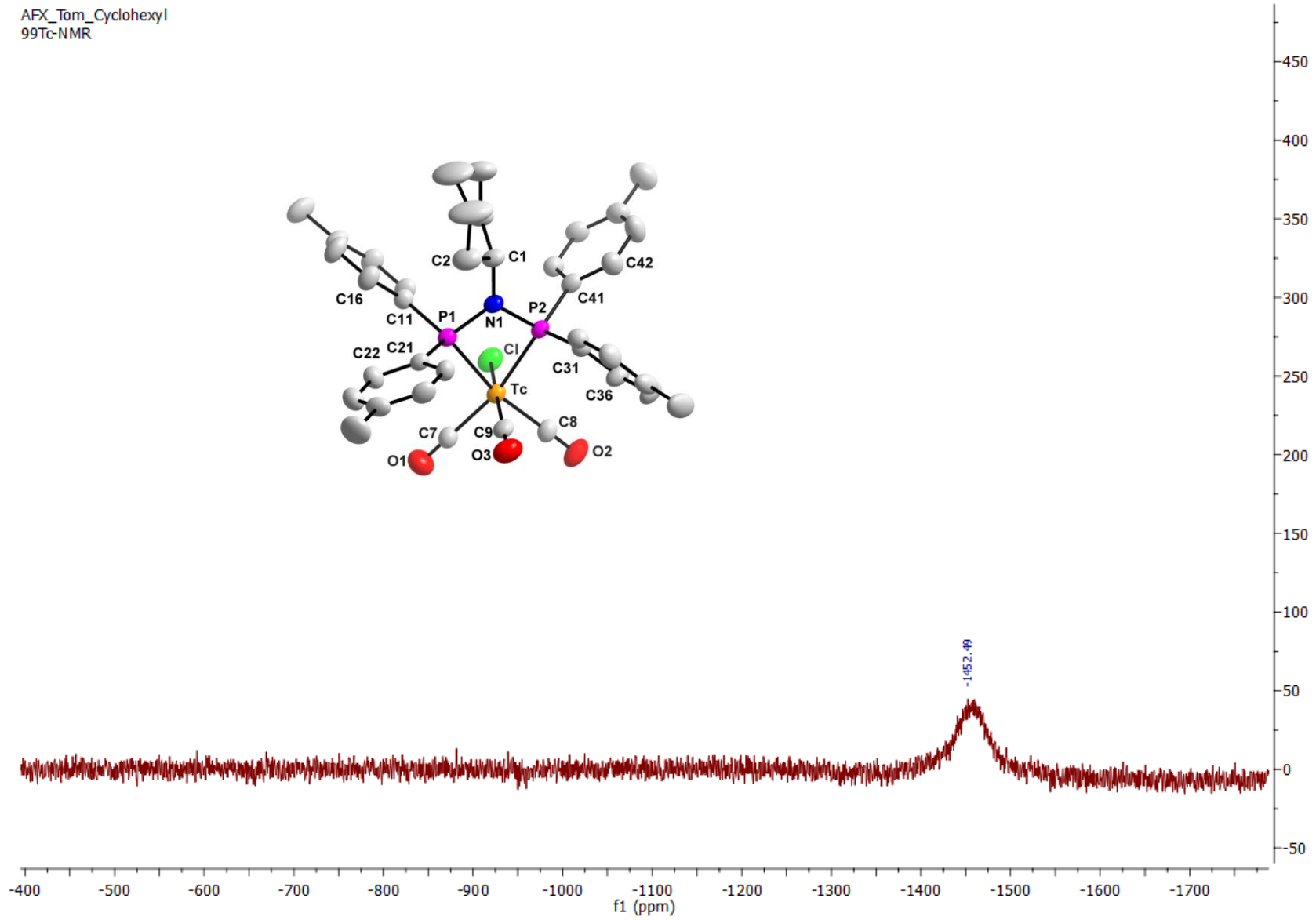

Figure S8 ^{31}P NMR spectrum for *fac*-[^{99}Tc(Cy-*p*TolPNP)(CO)$_3$Cl] (**1B**)

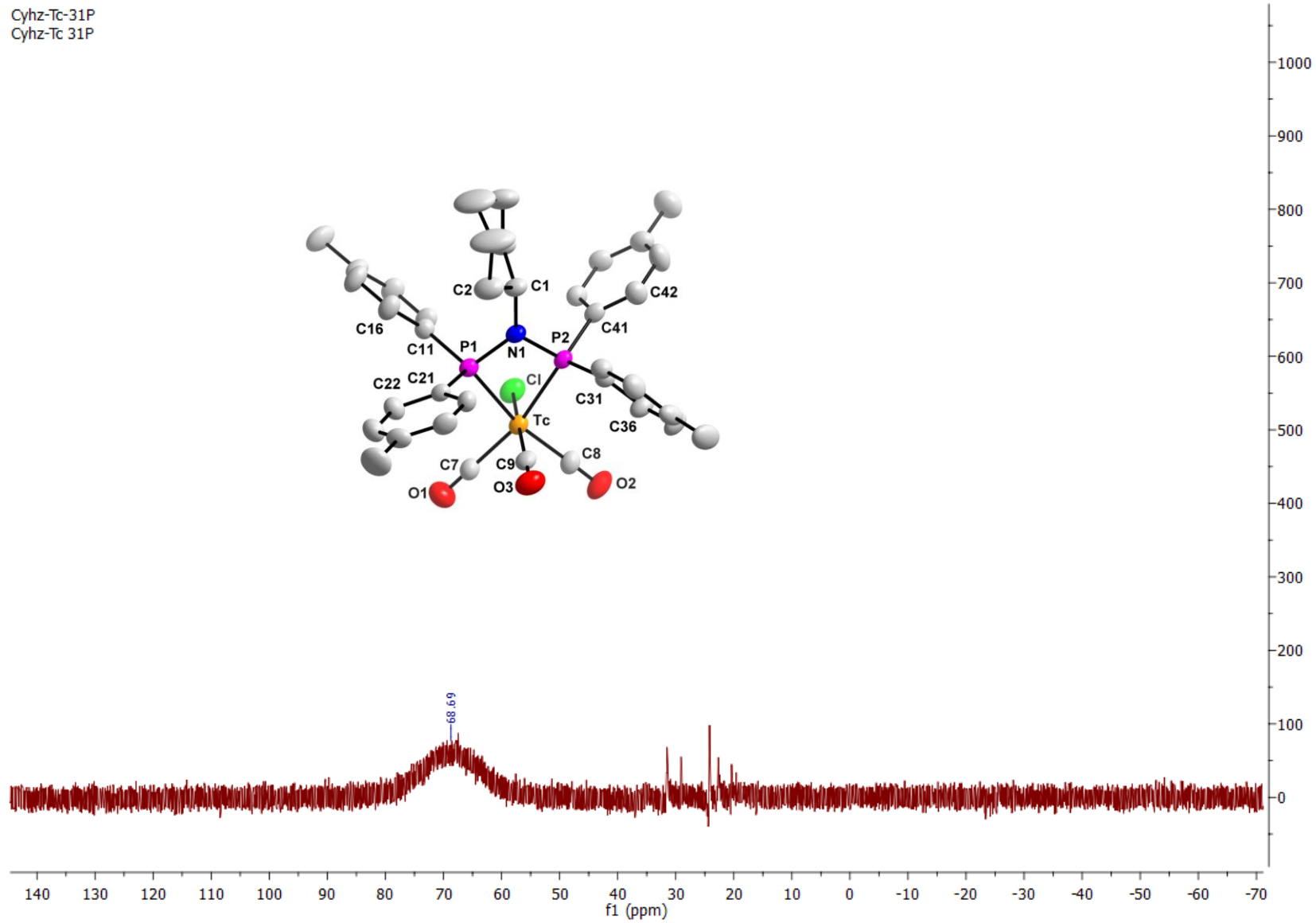

Figure S9 IR spectrum for *fac*-[^{99}Tc(Cy-*p*TolPNP)(CO)$_3$Cl] (**1B**) ATR

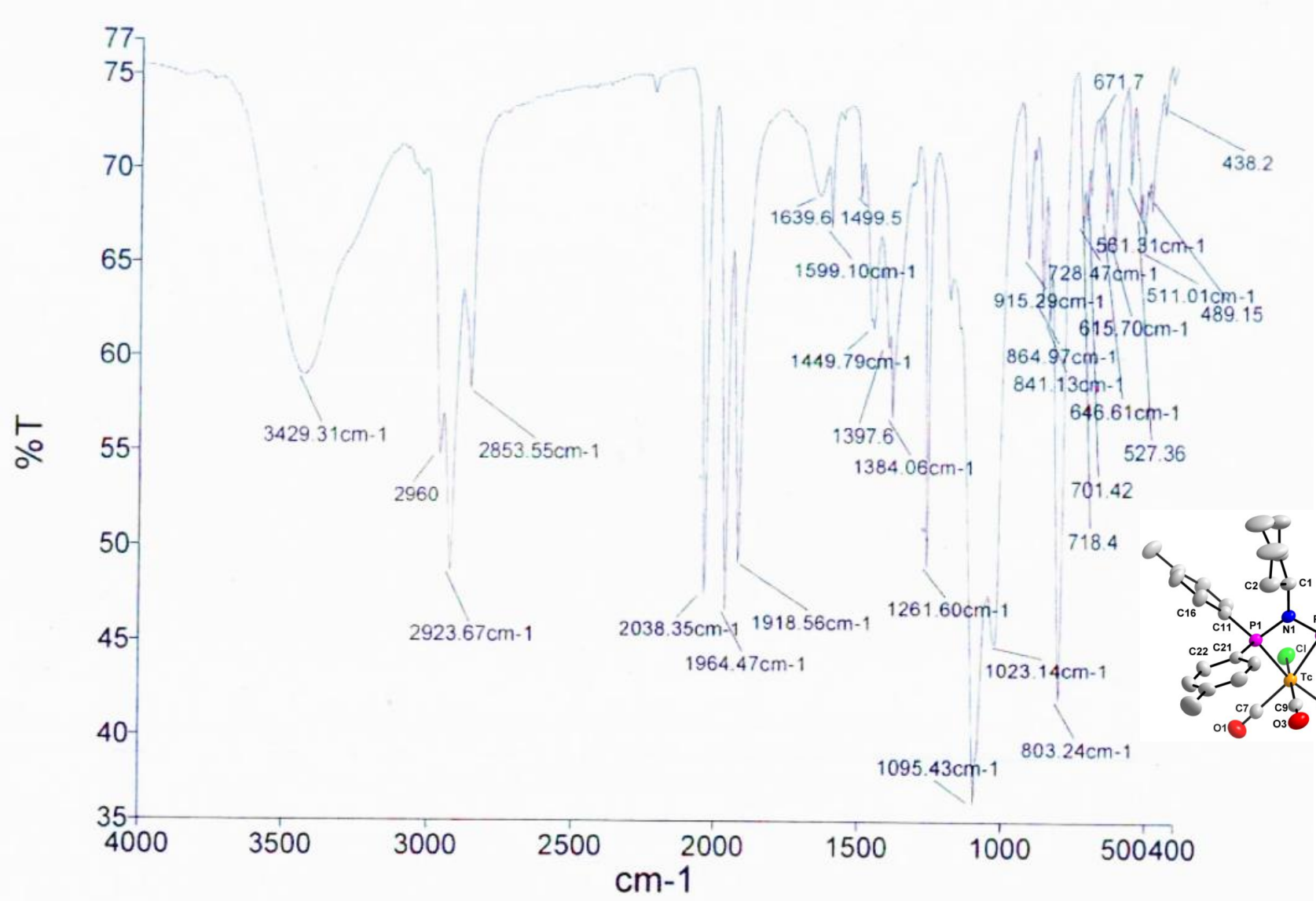

Figure S10 ^{1}H NMR spectrum for *fac*-[Re(Cb-*p*TolPNP)(CO)$_3$Br] (**2A**)

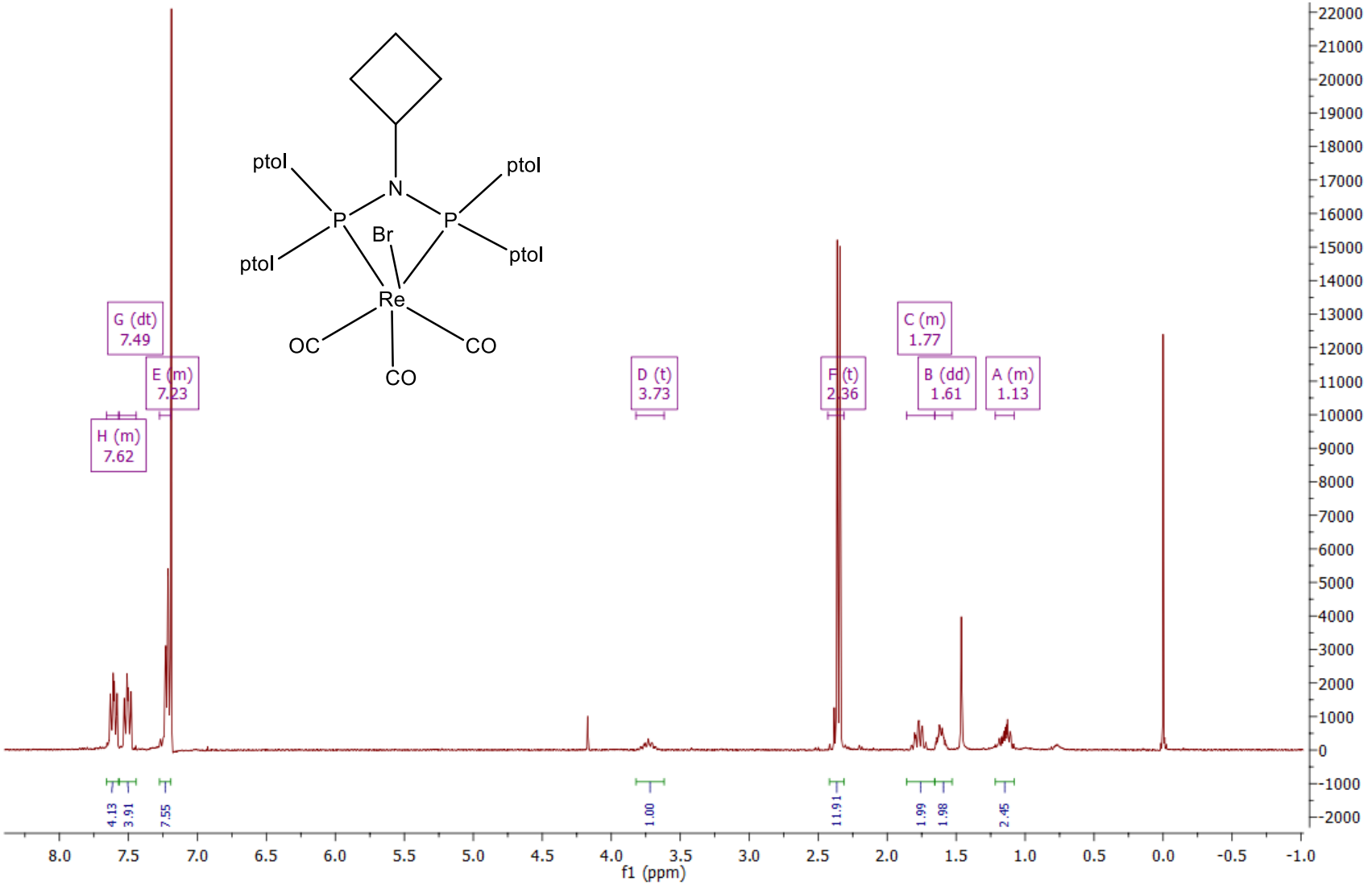

Figure S11 ^{31}P NMR spectrum for *fac*-[Re(Cb-*p*TolPNP)(CO)$_3$Br] (**2A**)

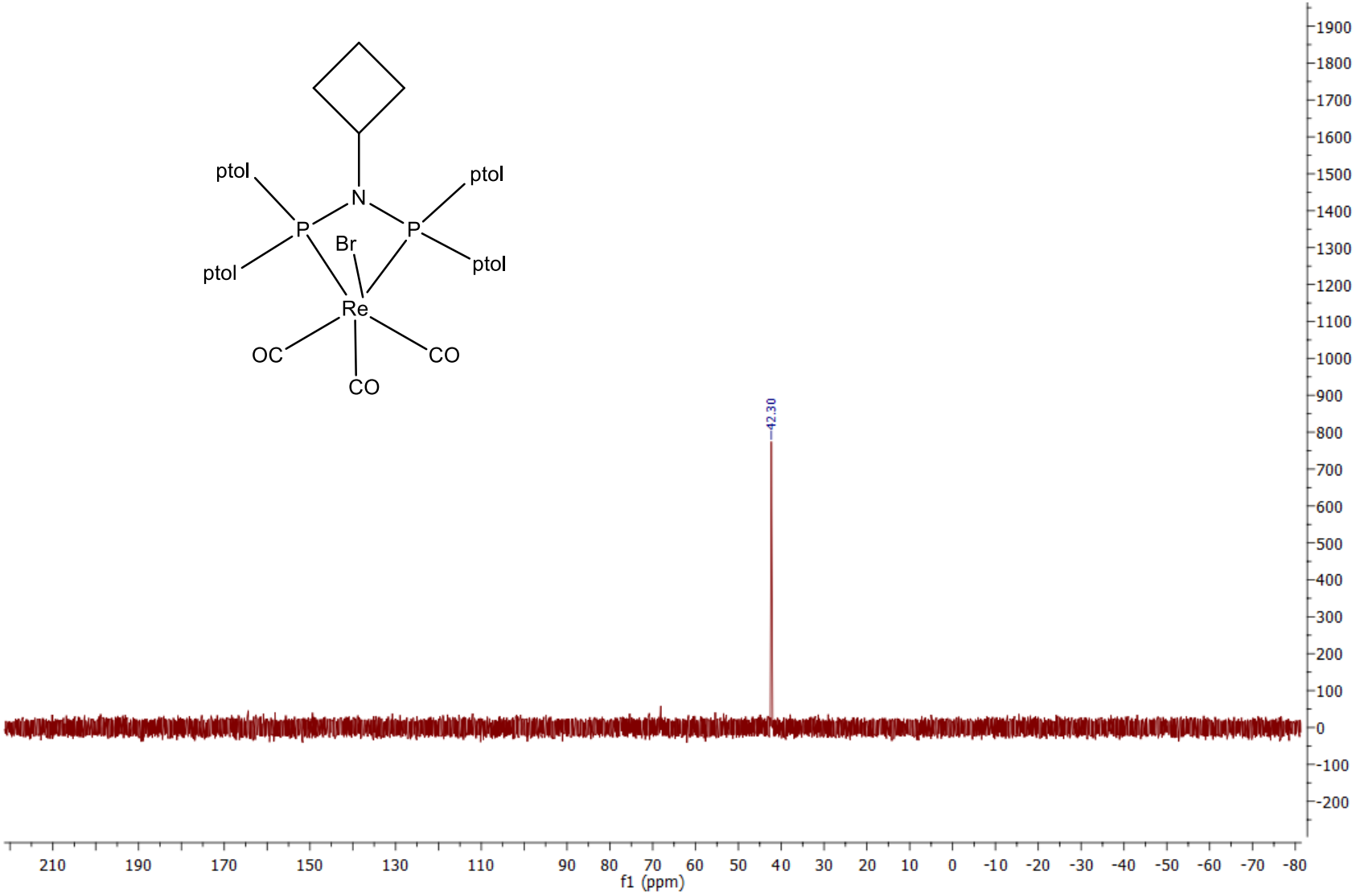

Figure S12 IR spectrum for *fac*-[Re(Cb-*p*TolPNP)(CO)$_3$Br] (**2A**) ATR

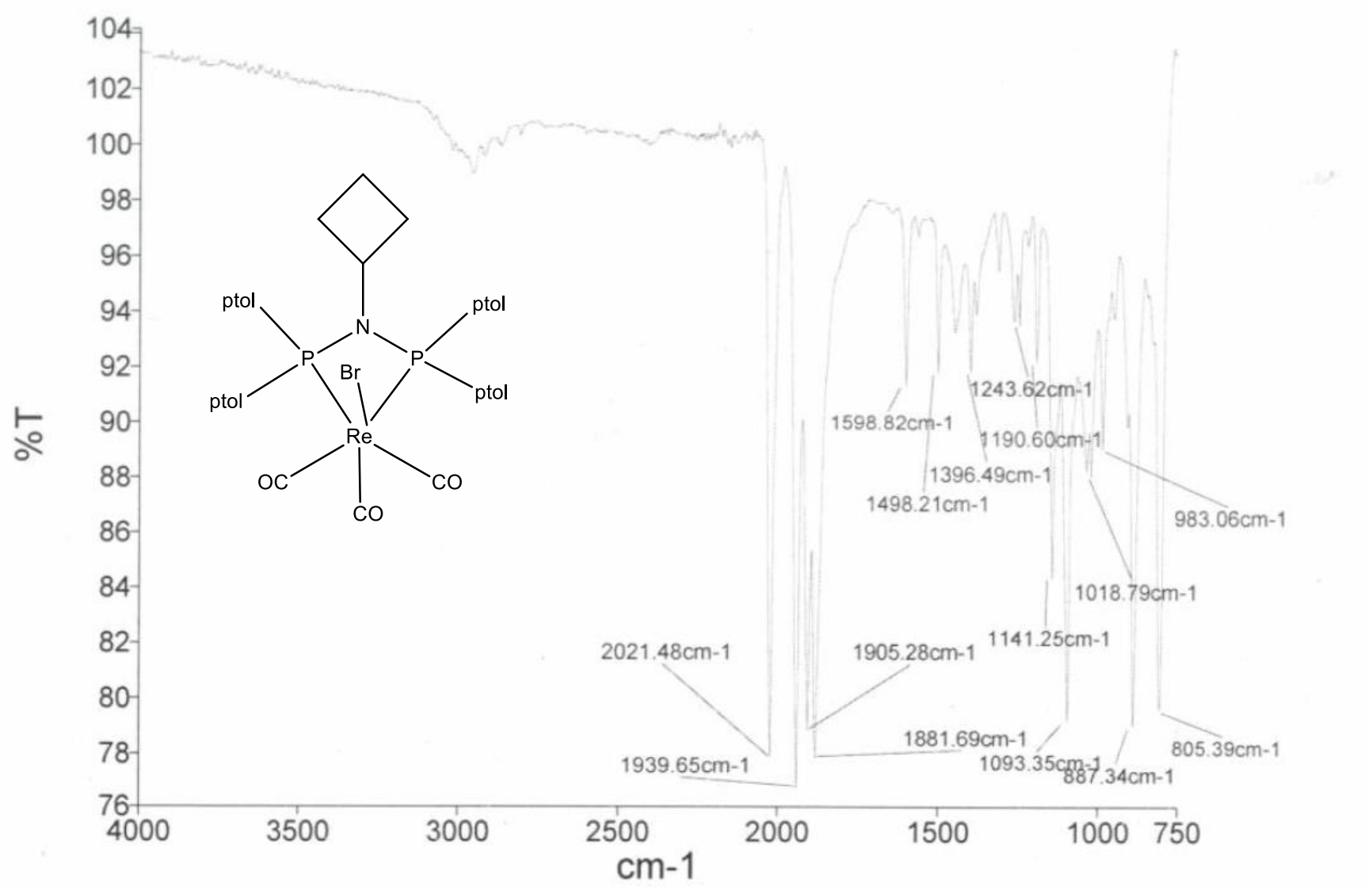

Figure S13 IR spectrum for *fac*-[Re(Cb-*p*TolPNP)(CO)$_3$Br] (**2A**) in DCM

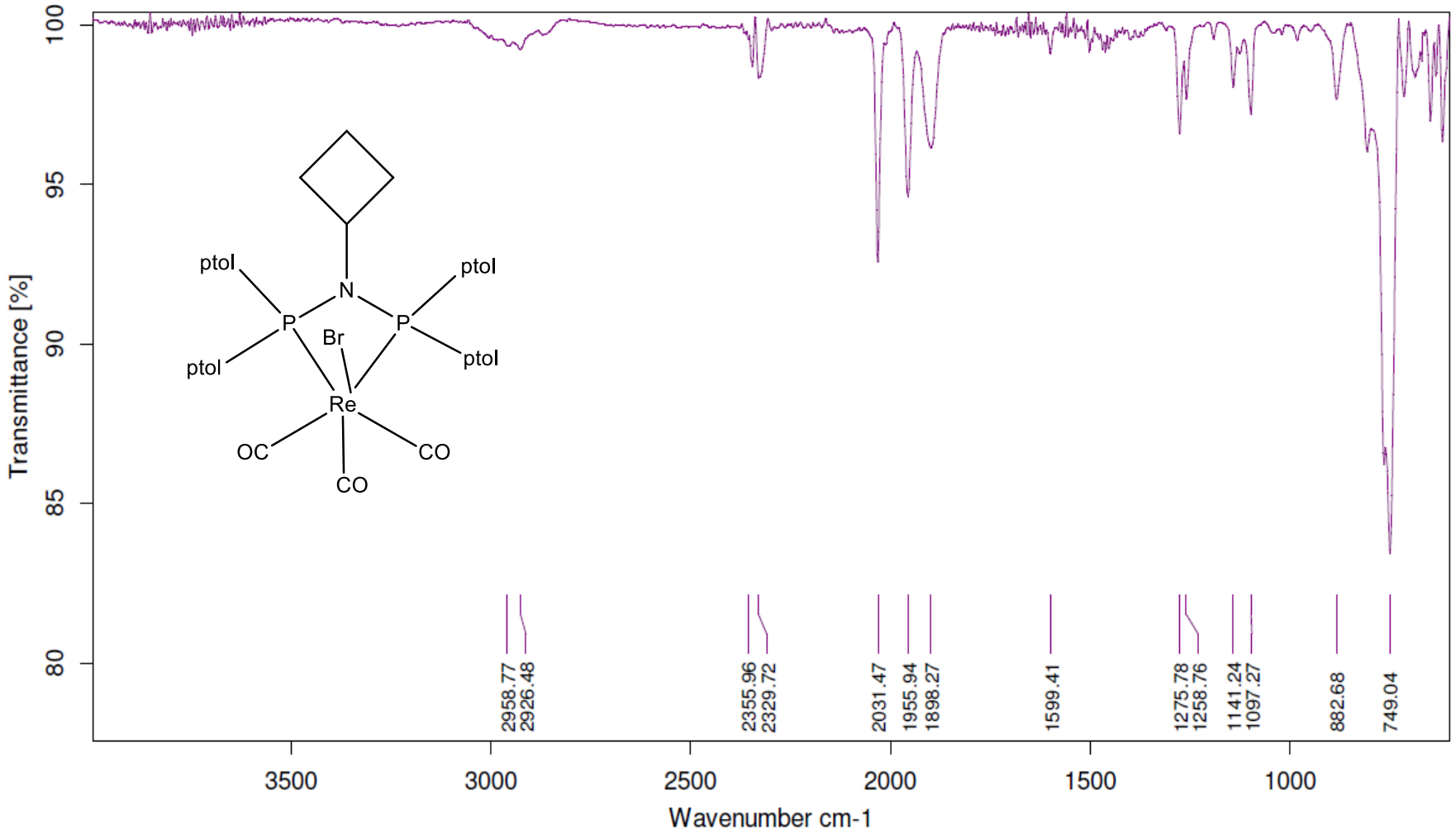

Figure S14 ^{1}H NMR spectrum for *fac*-[^{99}Tc(Cb-*p*TolPNP)(CO)$_3$Cl] (**2B**)

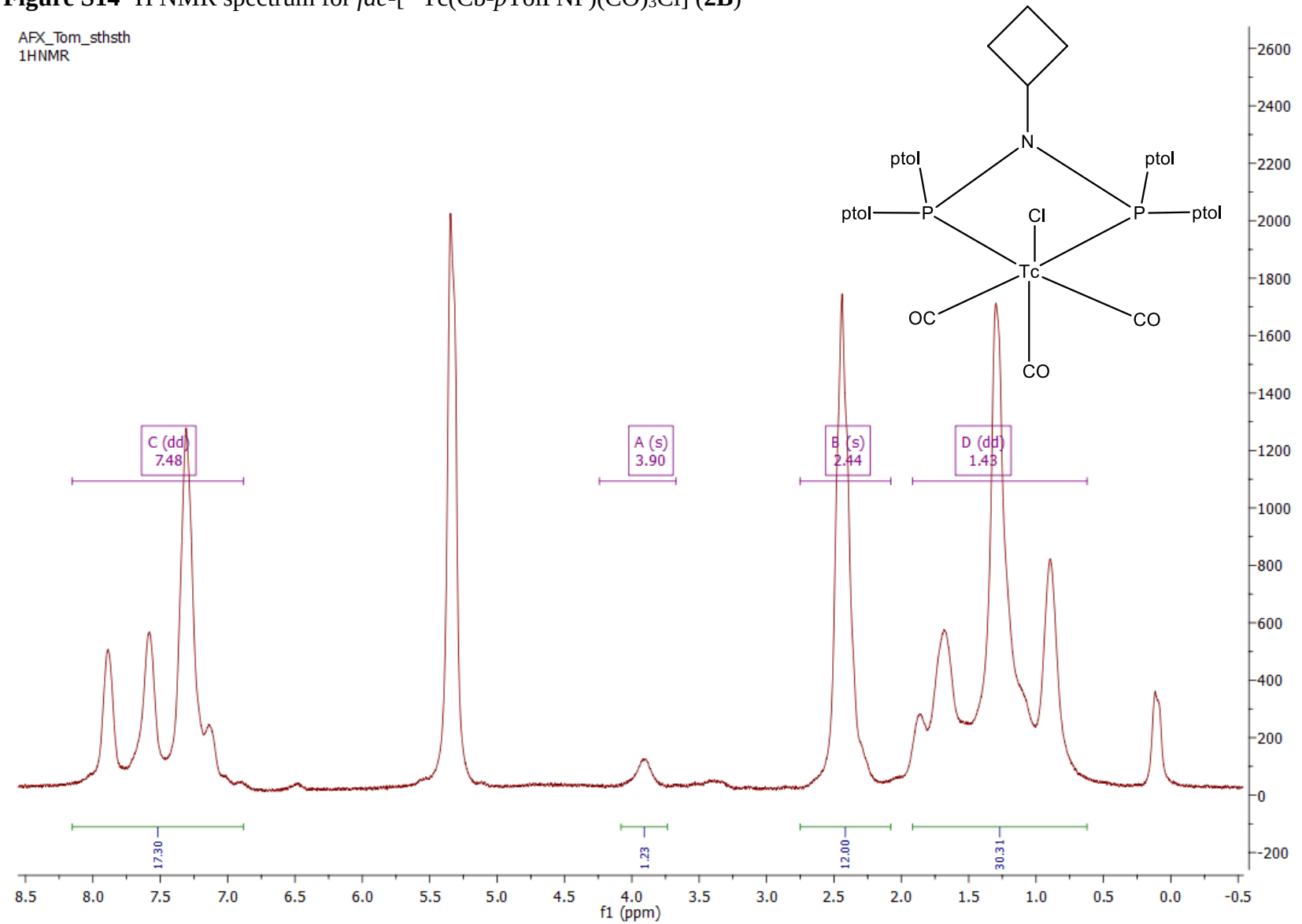

Figure S15 ^{99}Tc NMR spectrum for *fac*-[^{99}Tc(Cb-*p*TolPNP)(CO)$_3$Cl] (**2B**)

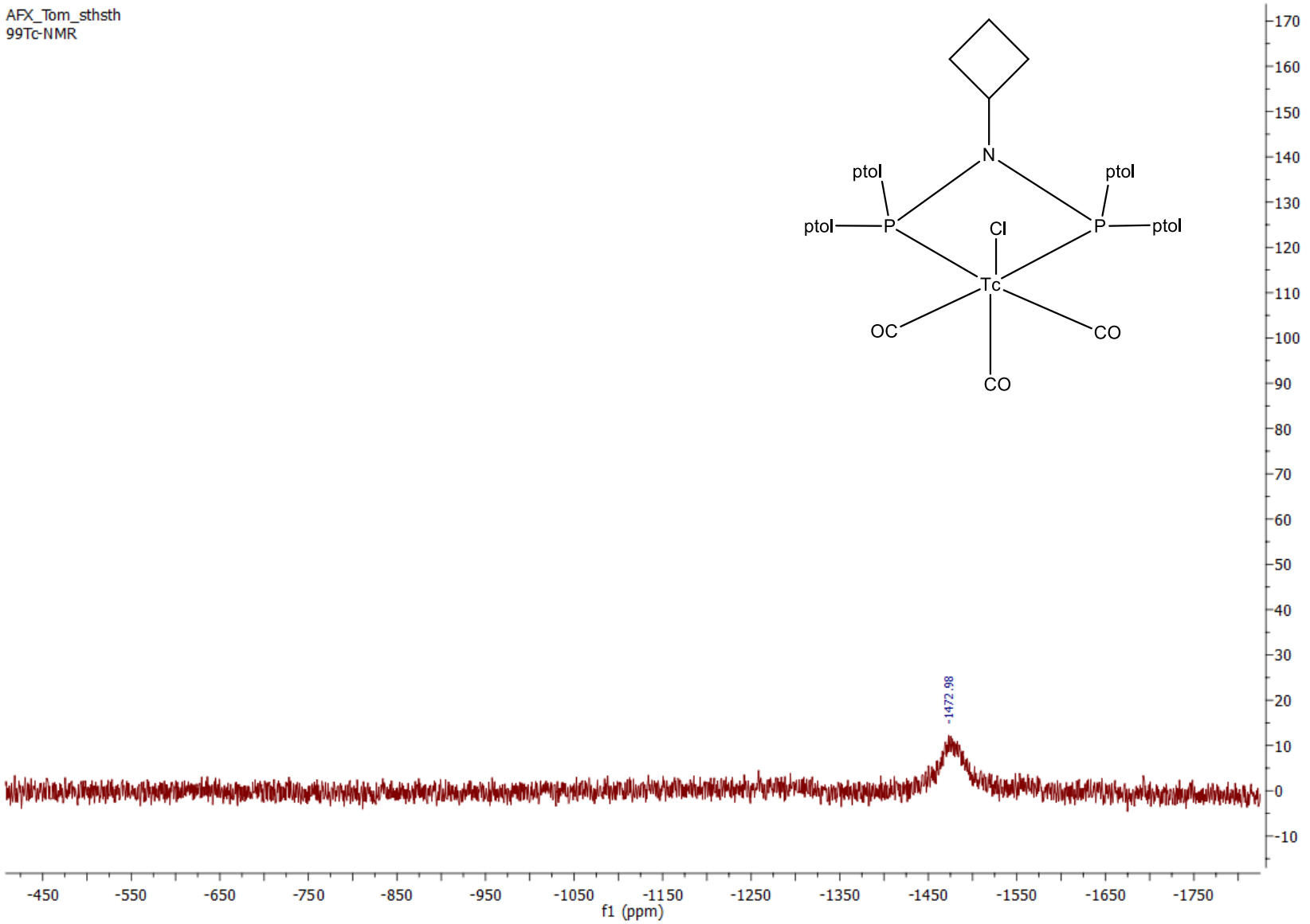

Figure S16 ^{31}P NMR spectrum for *fac*-[^{99}Tc(Cb-*p*TolPNP)(CO)$_3$Cl] (**2B**)

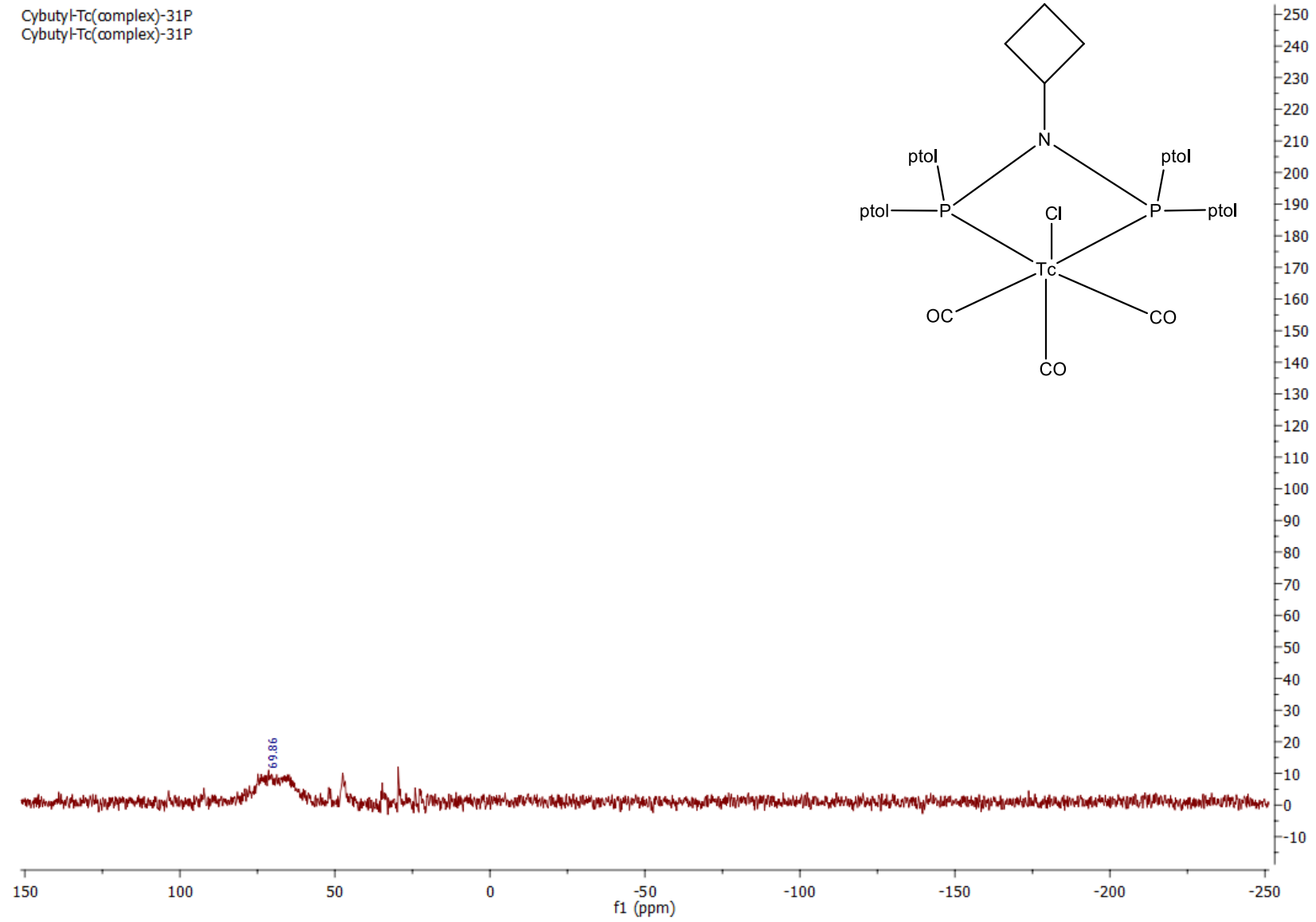

Figure S17 IR spectrum for *fac*-[^{99}Tc(Cb-*p*TolPNP)(CO)$_3$Cl] (**2B**)

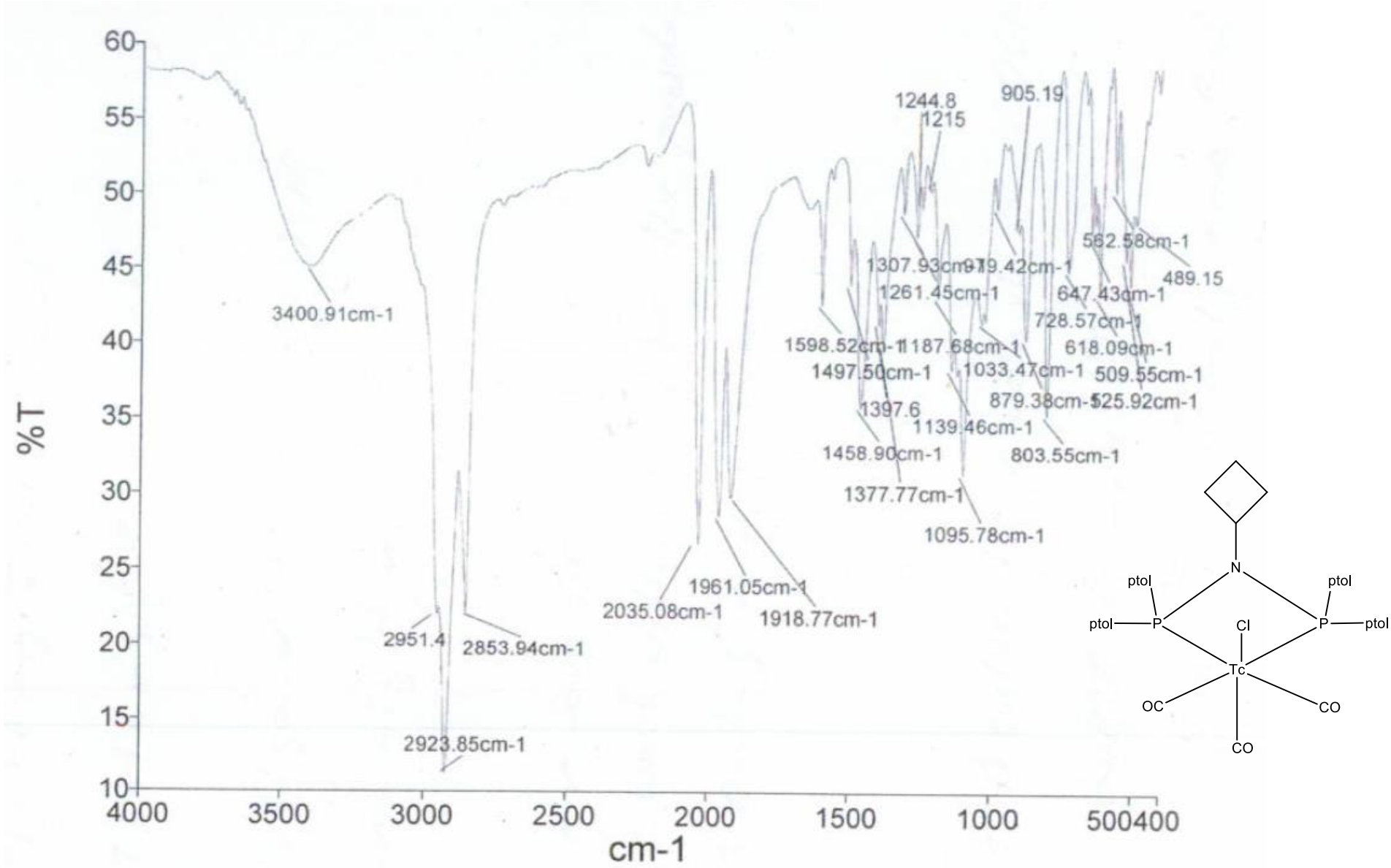

Figure S18 ^{1}H NMR spectrum for Chzyl-4-*p*tol-PNP (**1**)

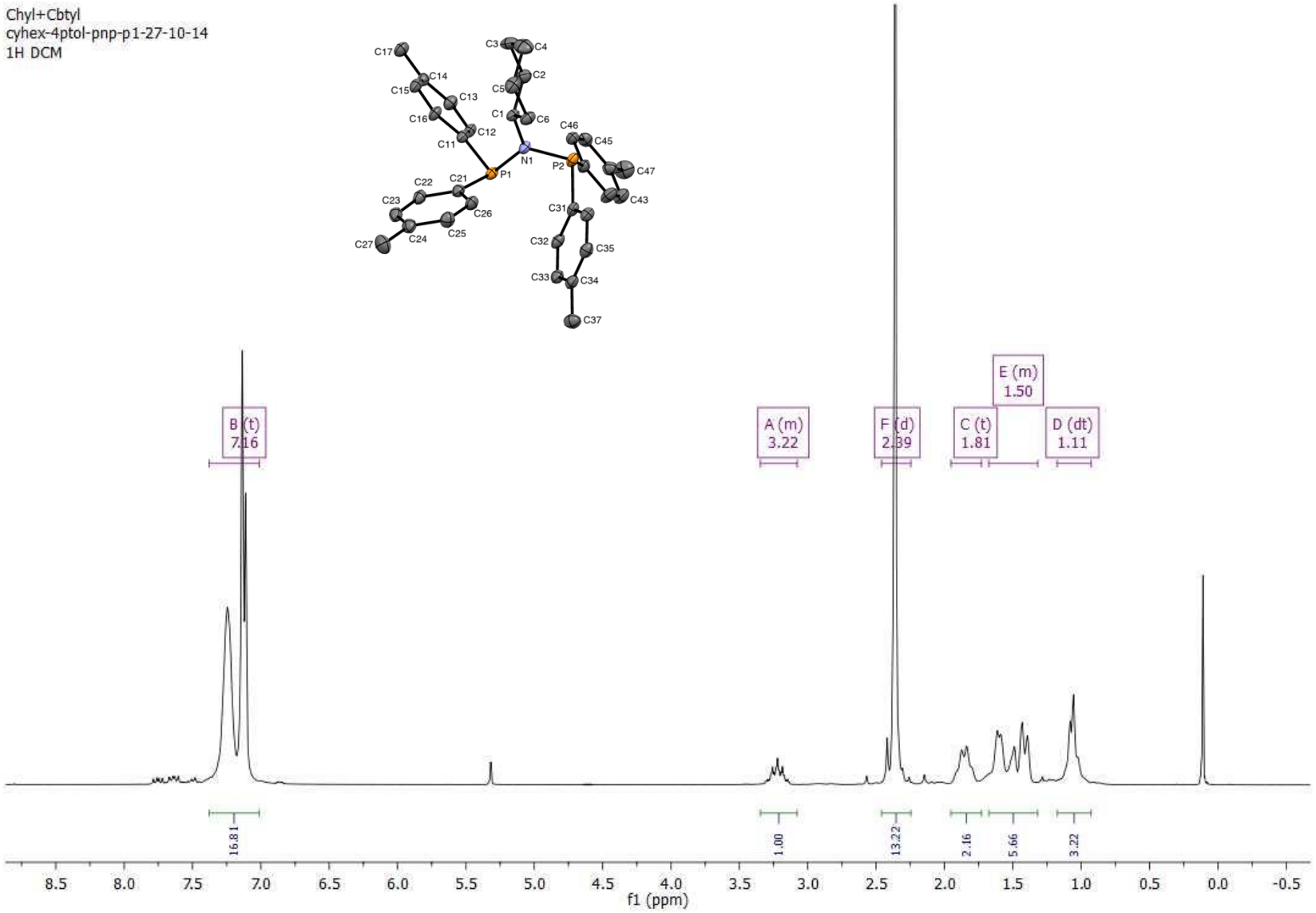

Figure S19 ^{31}P NMR spectrum for Chzyl-4*p*tol-PNP (**1**)

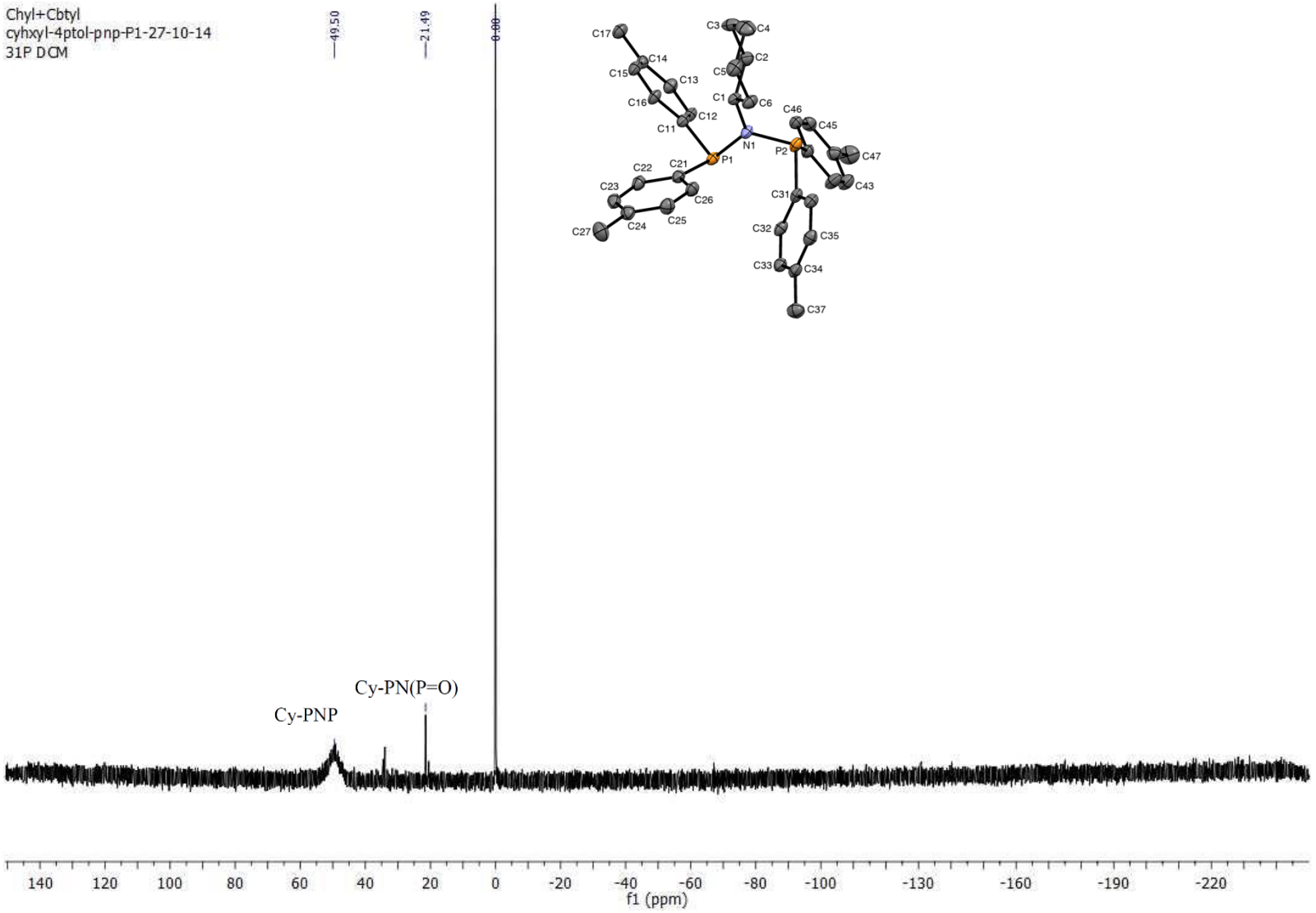

Figure S20 ^{1}H NMR spectrum for Cyclobutyl-4*p*tol-PNP (**2**)

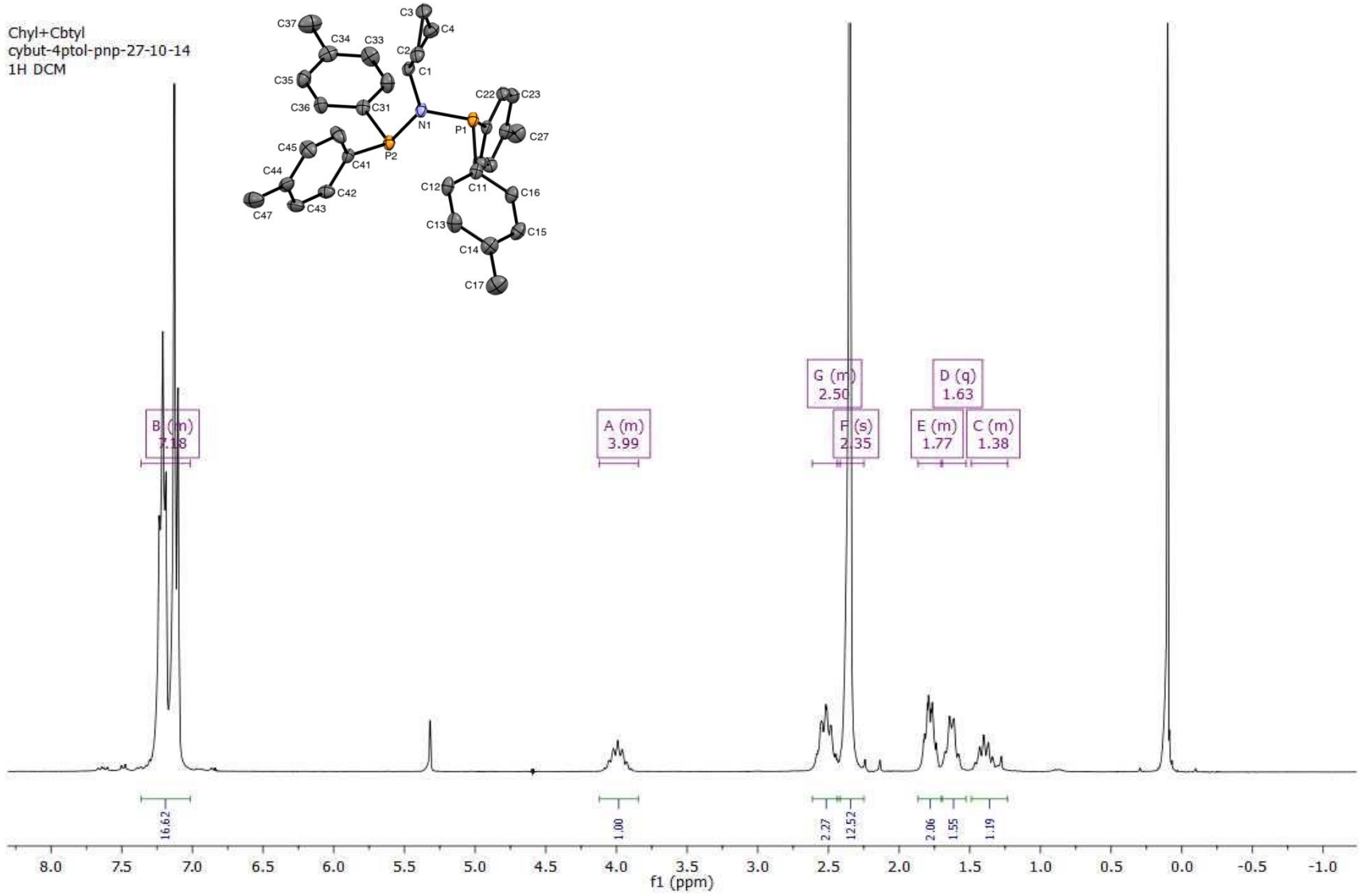

Figure S21 ^{31}P NMR spectrum for Cyclobutyl-4*p*tol-PNP (**2**)

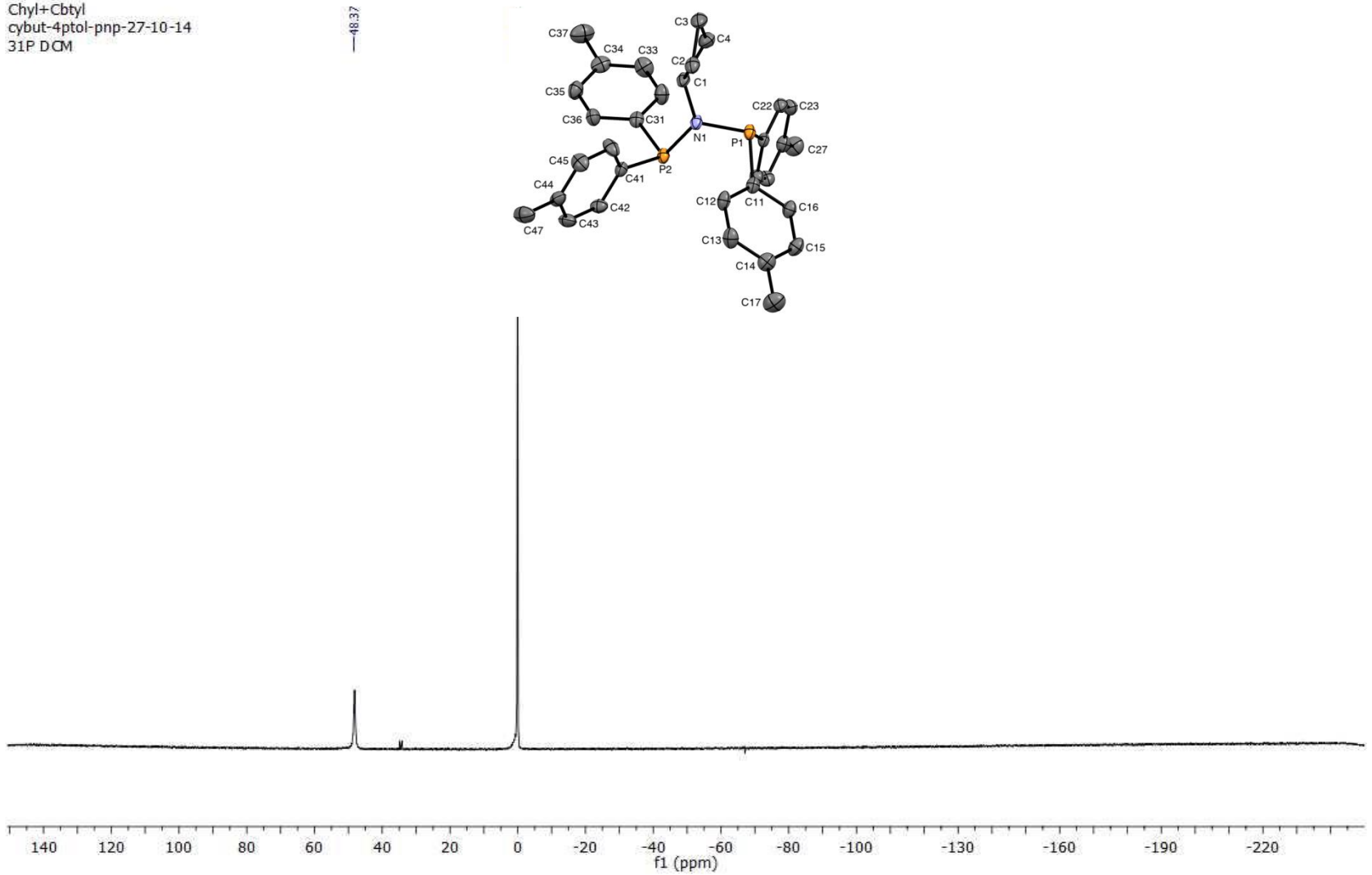

Figure S22 Illustration of (a) disorder in **1**, yielding (b) ca. 80% of the unoxidized Cy-PNP ligand, and (c) ca. 20% of the mono-oxidized product, Cy-PN(P=O)