Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Titanium Isopropoxide Complexes of a Series of Sterically Demanding Aryloxo Based $[N_2O_2]^{2-}$ Ligands as Precatalysts for Ethylene Polymerization

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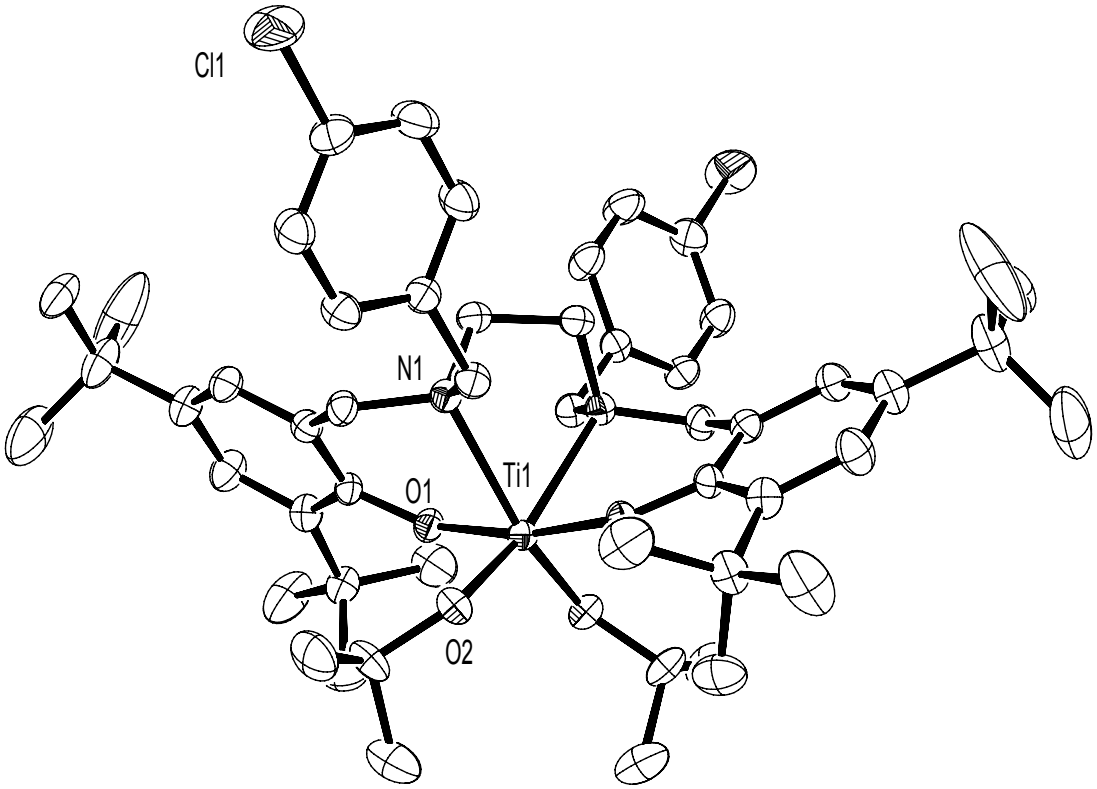


Figure S1. ORTEP view of the solid state structure of **5b**. The thermal ellipsoids are shown in 50 % probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°) are given: Ti1-O1 1.887(2), Ti1-O2 1.823(2), Ti1-N1 2.401(3), O1-Ti1-O2 91.37(10), O1-Ti1-N1 90.86(10), O2-Ti1-N1 89.36(10).

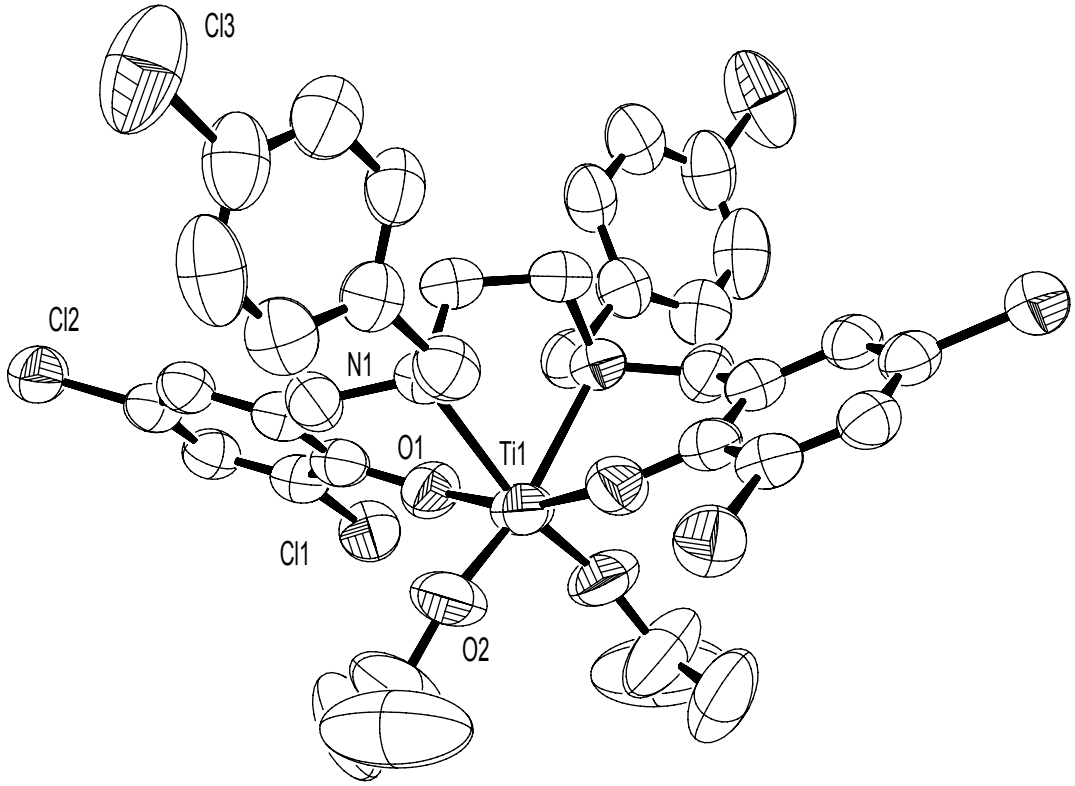


Figure S2. ORTEP view of the solid state structure of **6b**. The thermal ellipsoids are shown in 50 % probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°) are given: Ti1-O1 1.909(4), Ti1-O2 1.767(4), Ti1-N1 2.354(4), O1-Ti1-O2 96.81(19), O2-Ti1-N1 164.39(17), O1-Ti1-N1 85.56(16).

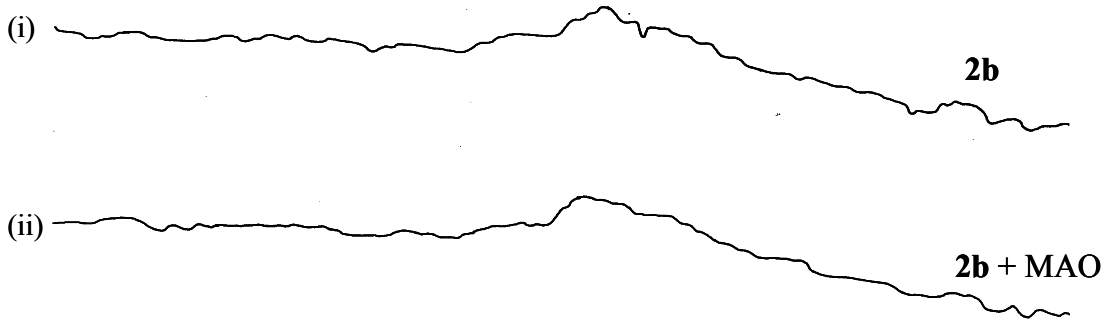


Figure S3. ESR spectrum (i) of the complex **2b** and (ii) of the complex **2b** when activated by MAO and both recorded at 77 K.

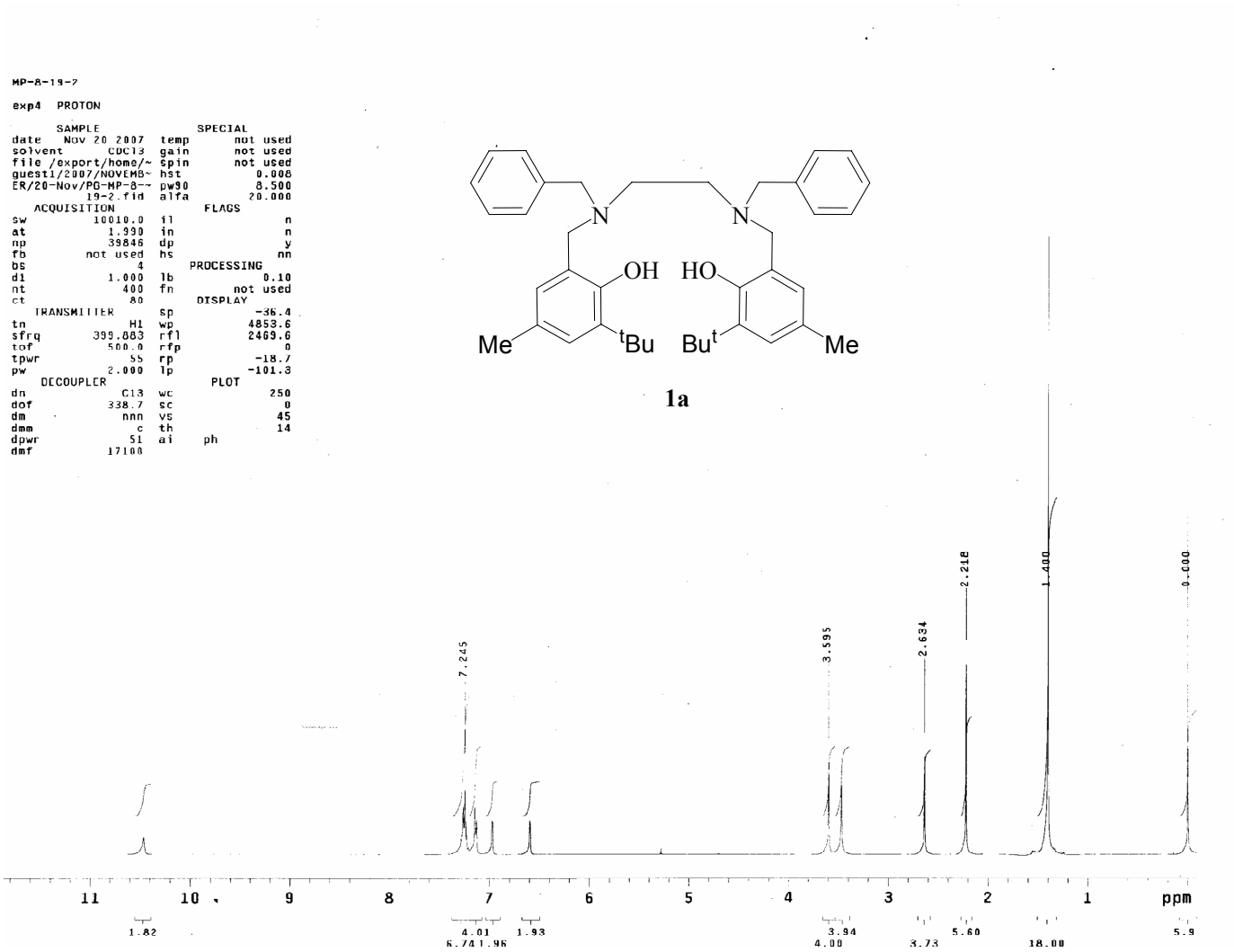
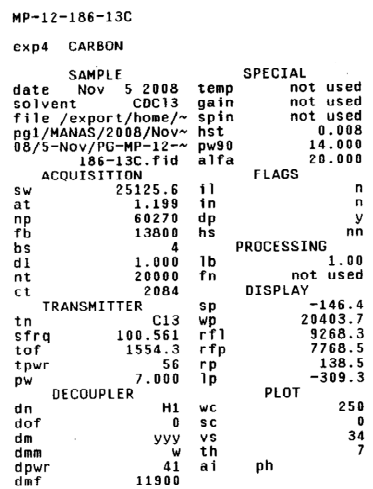
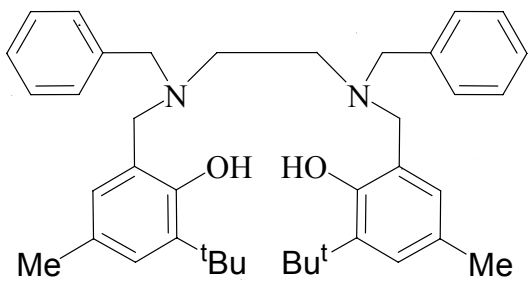


Figure S4. ^{1}H NMR spectrum of **1a** in $CDCl_3$.





1a

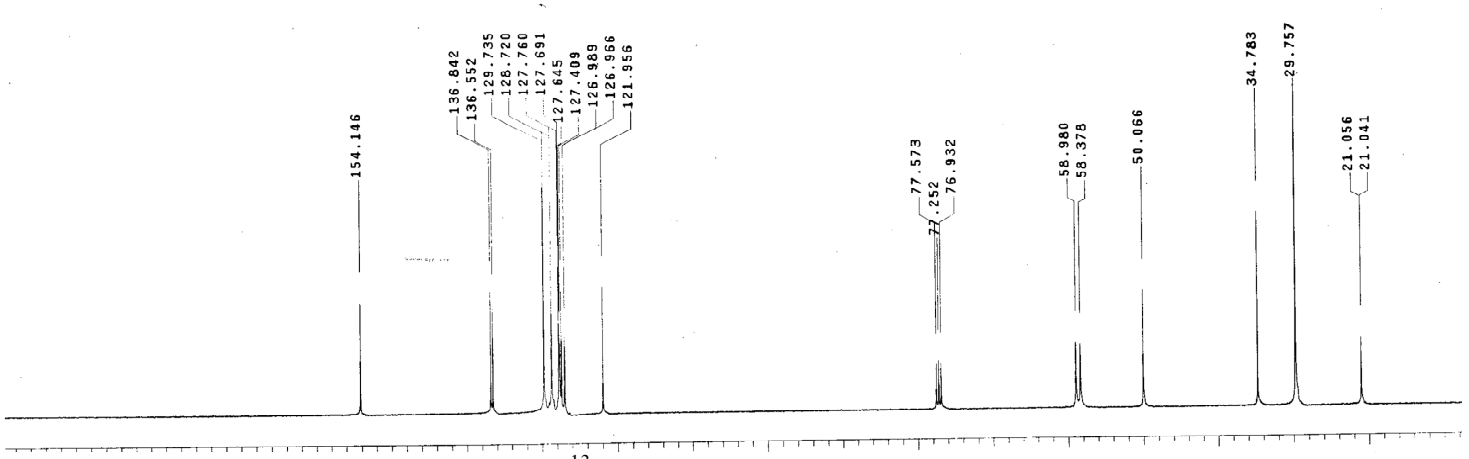


Figure S5. ^{13}C NMR spectrum of **1a** in $CDCl_3$.

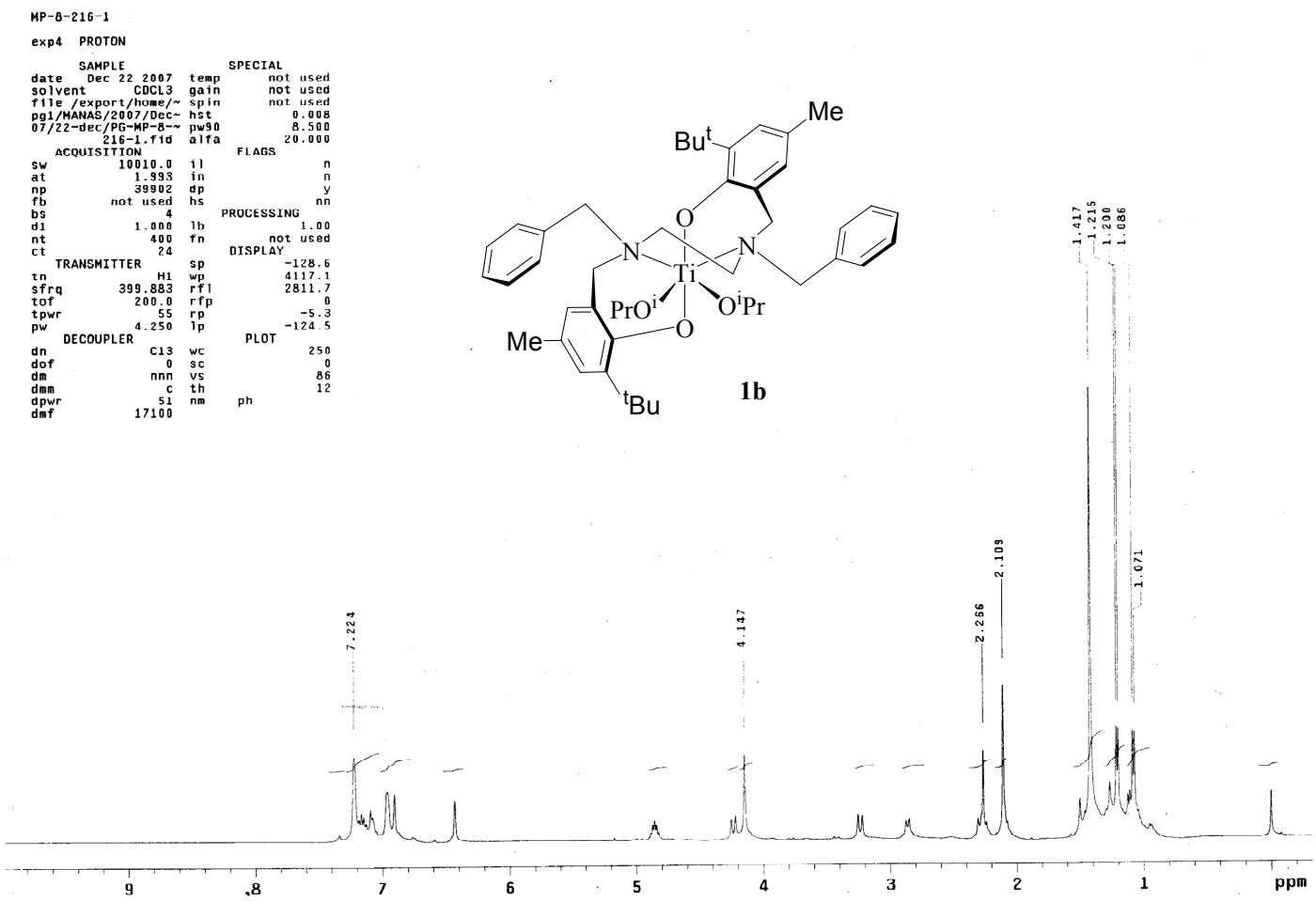


Figure S6. ^{1}H NMR spectrum of **1b** in $CDCl_3$.

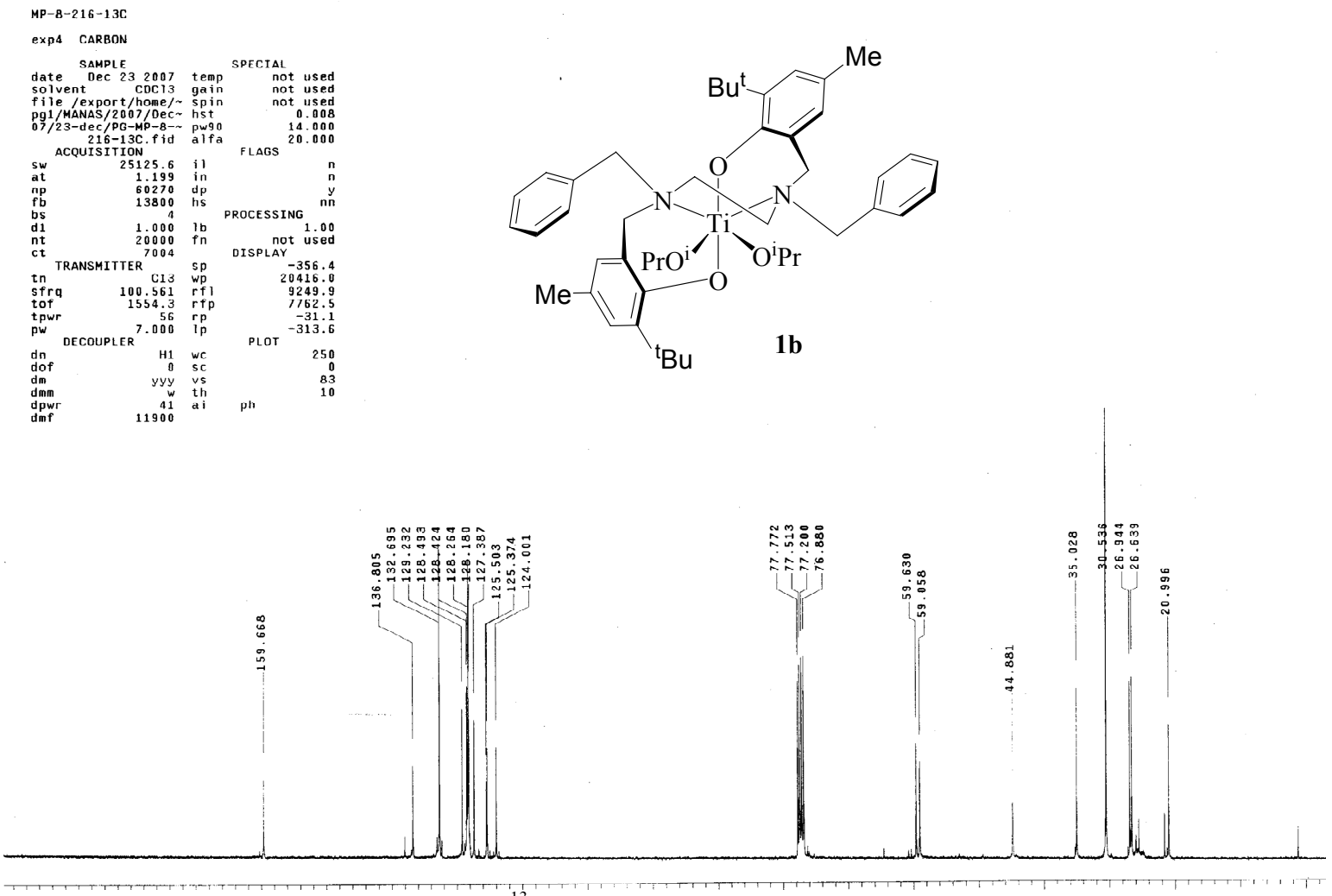


Figure S7. ^{13}C NMR spectrum of **1b** in $CDCl_3$.

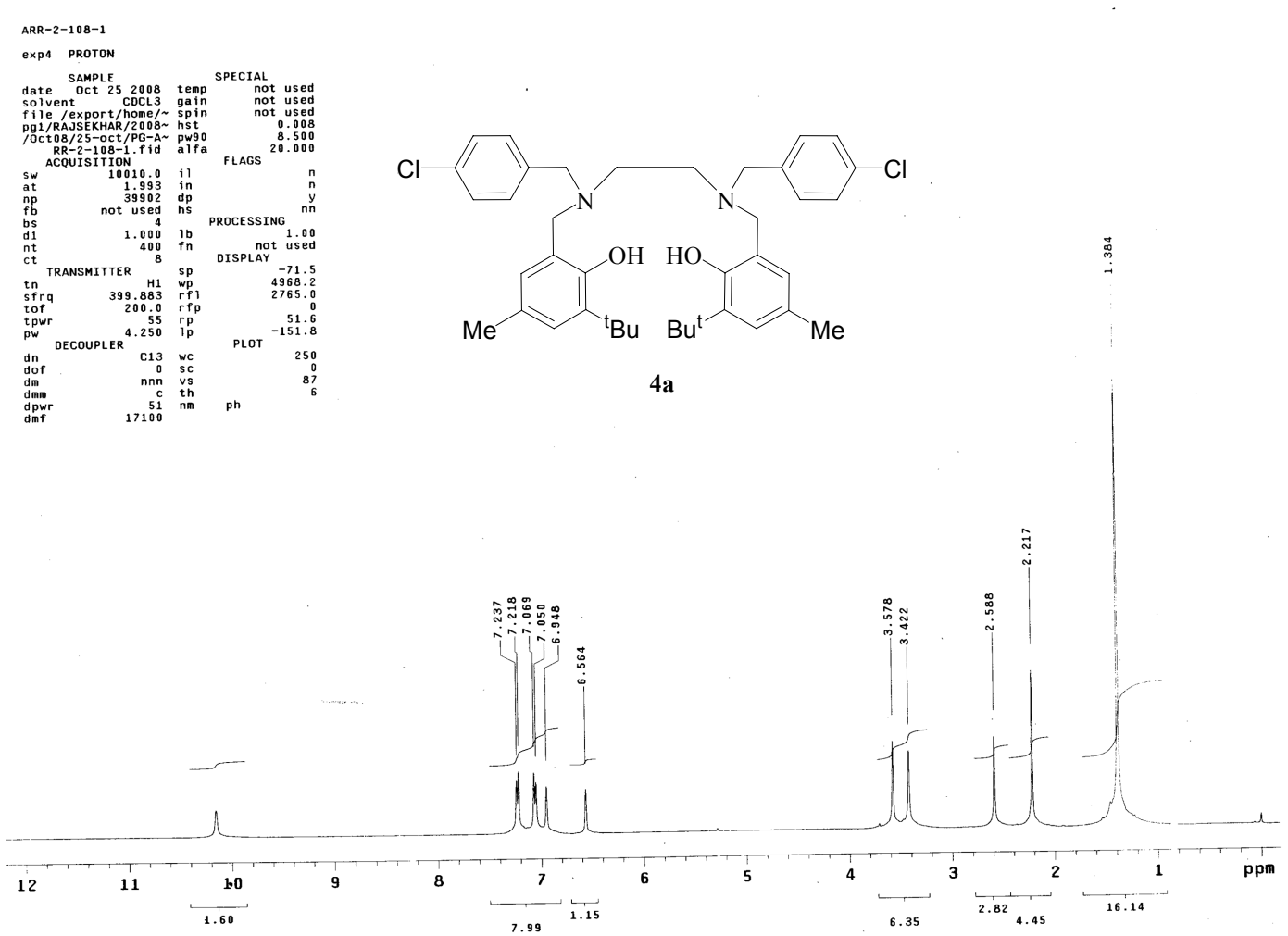


Figure S8. ^{1}H NMR spectrum of **4a** in $CDCl_3$.

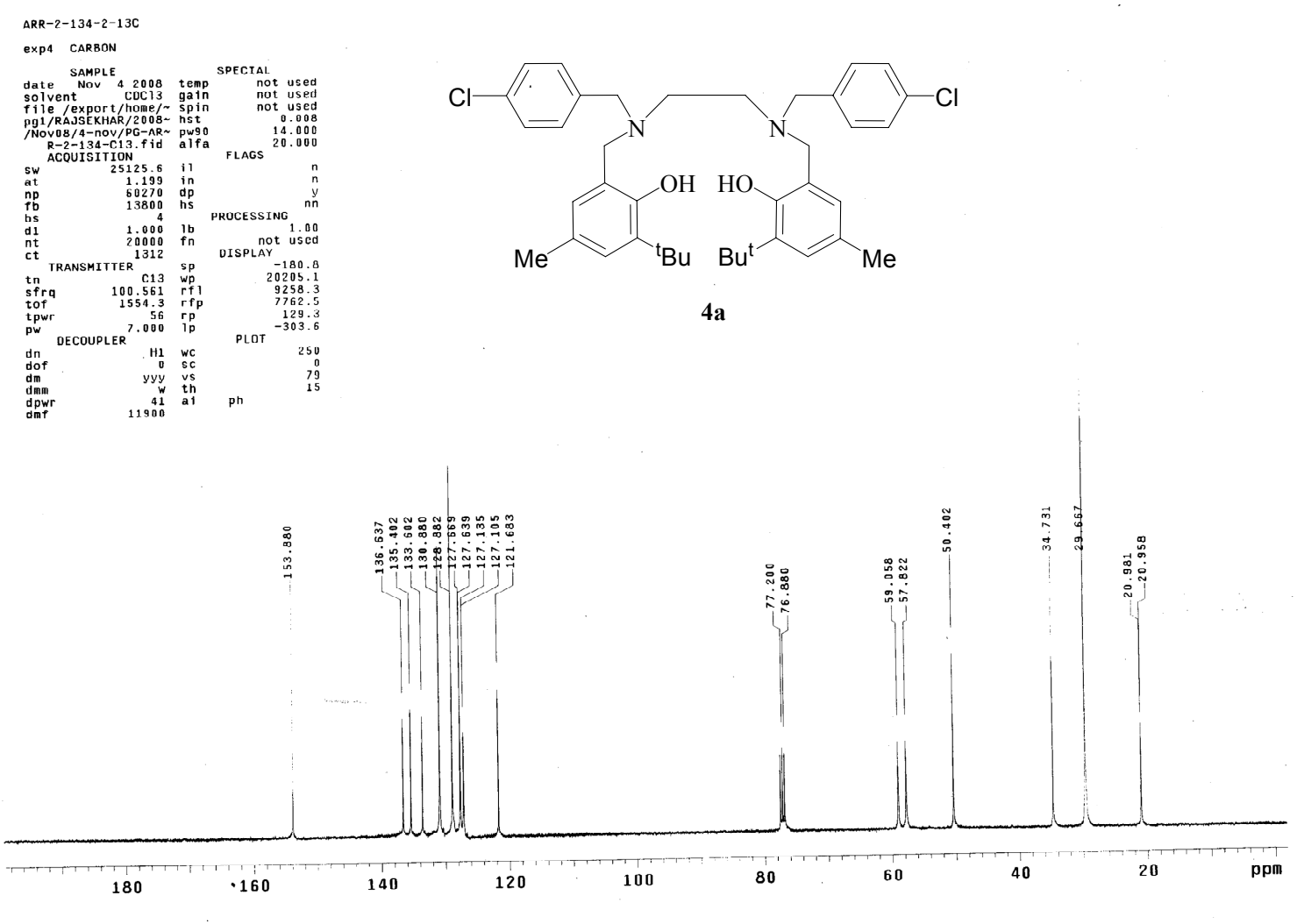


Figure S9. ^{13}C NMR spectrum of **4a** in $CDCl_3$.

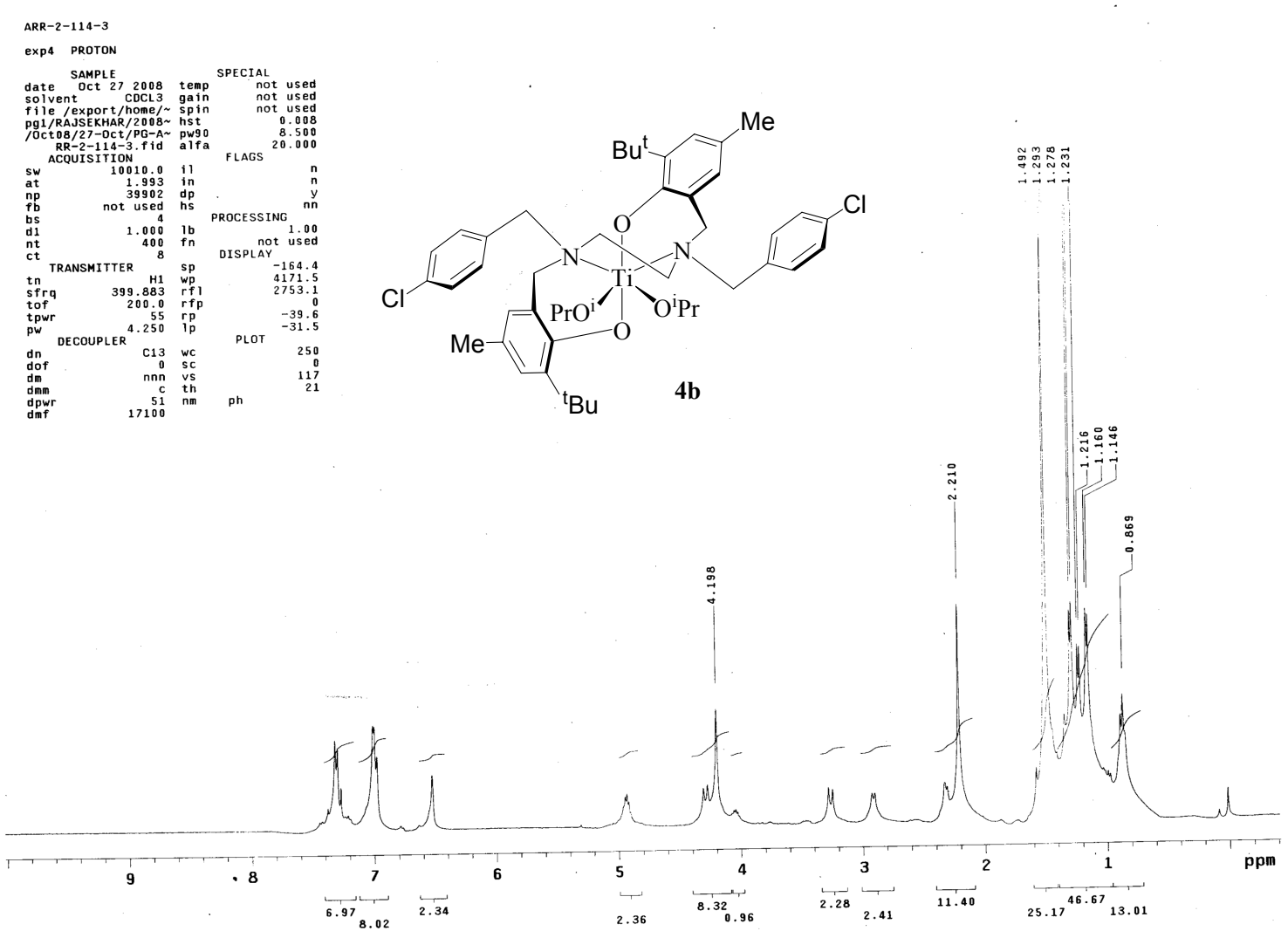


Figure S10. ^{1}H NMR spectrum of **4b** in $CDCl_3$.

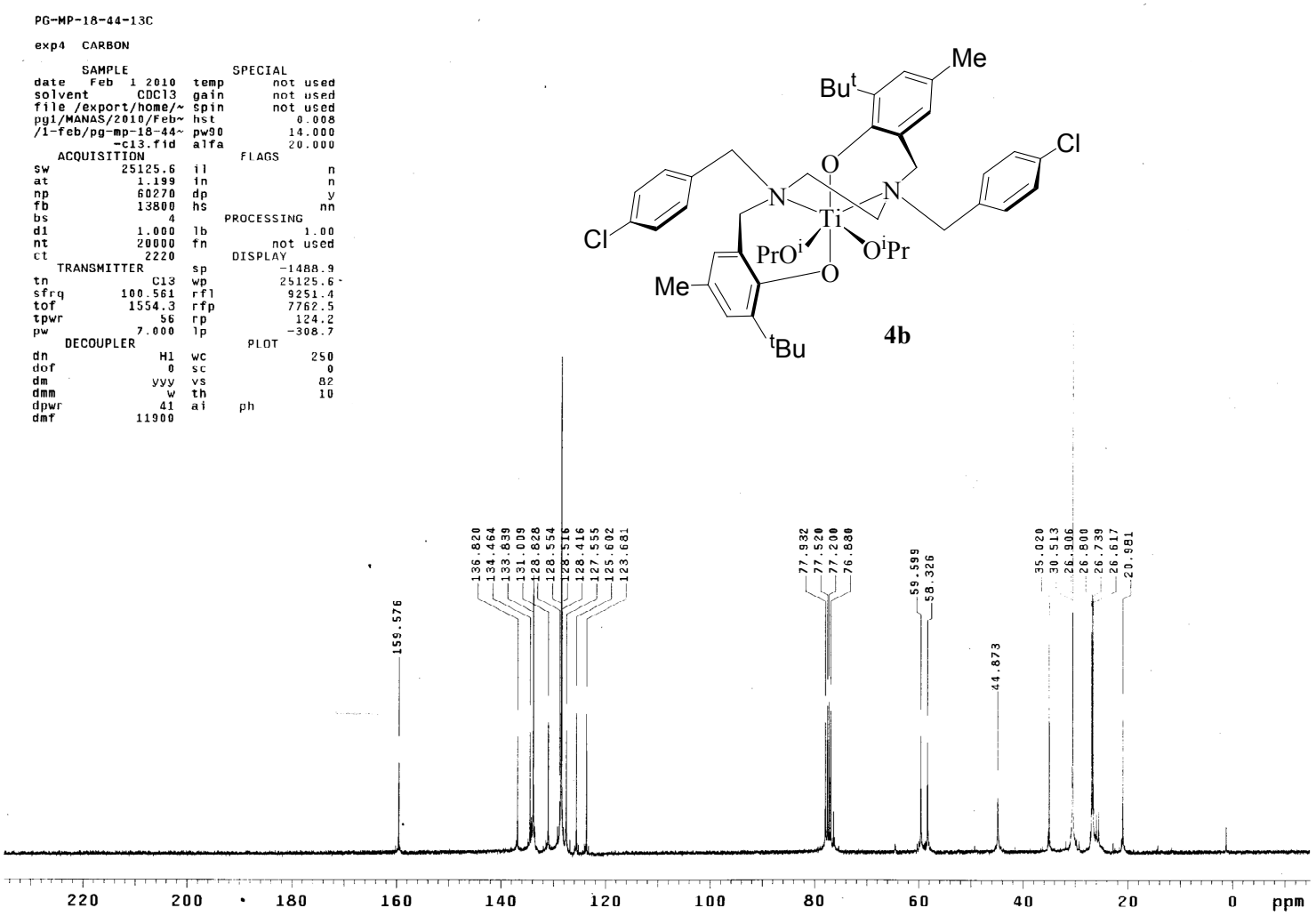


Figure S11. ^{13}C NMR spectrum of **4b** in $CDCl_3$.

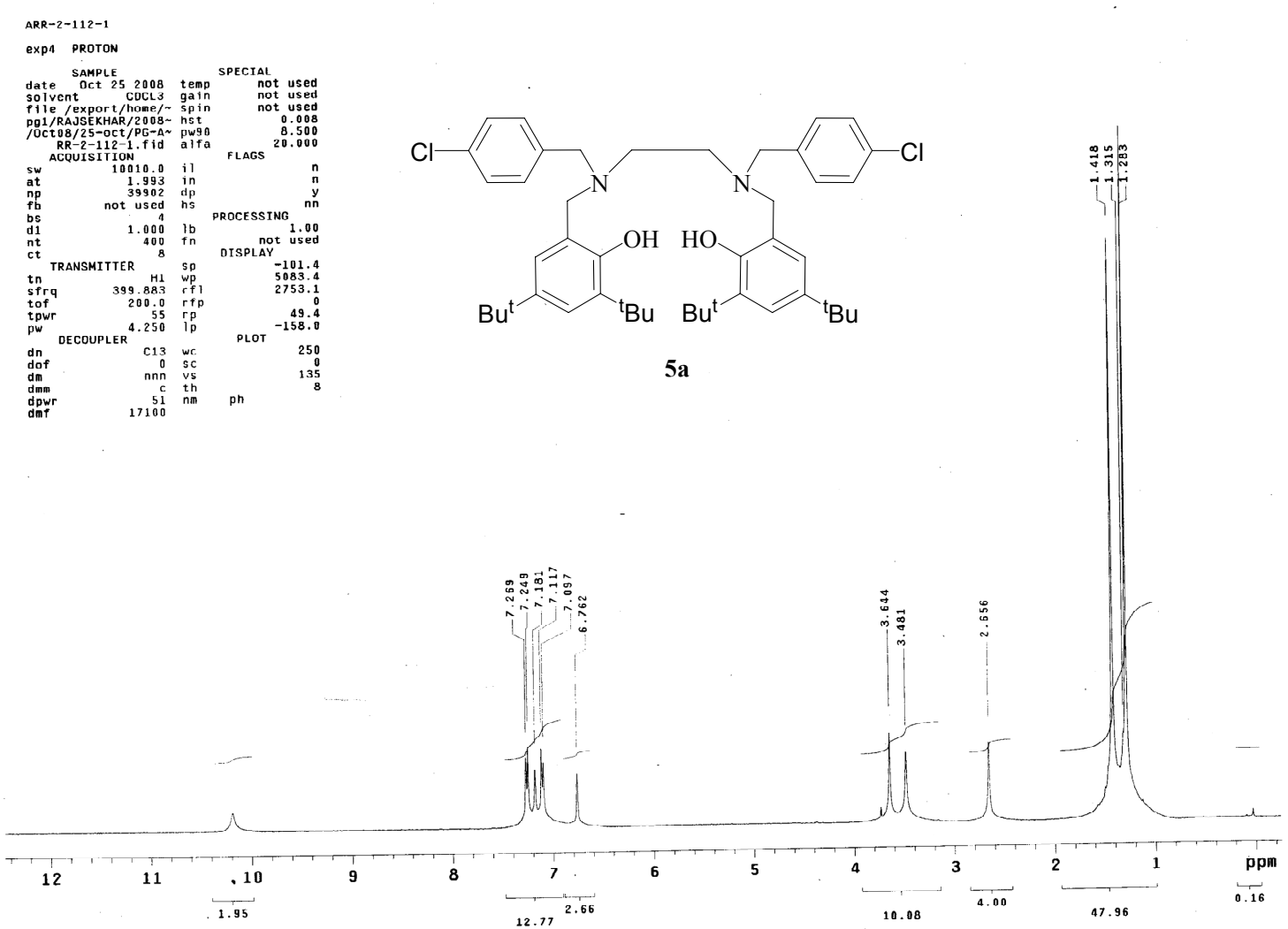


Figure S12. ^{1}H NMR spectrum of **5a** in $CDCl_3$.

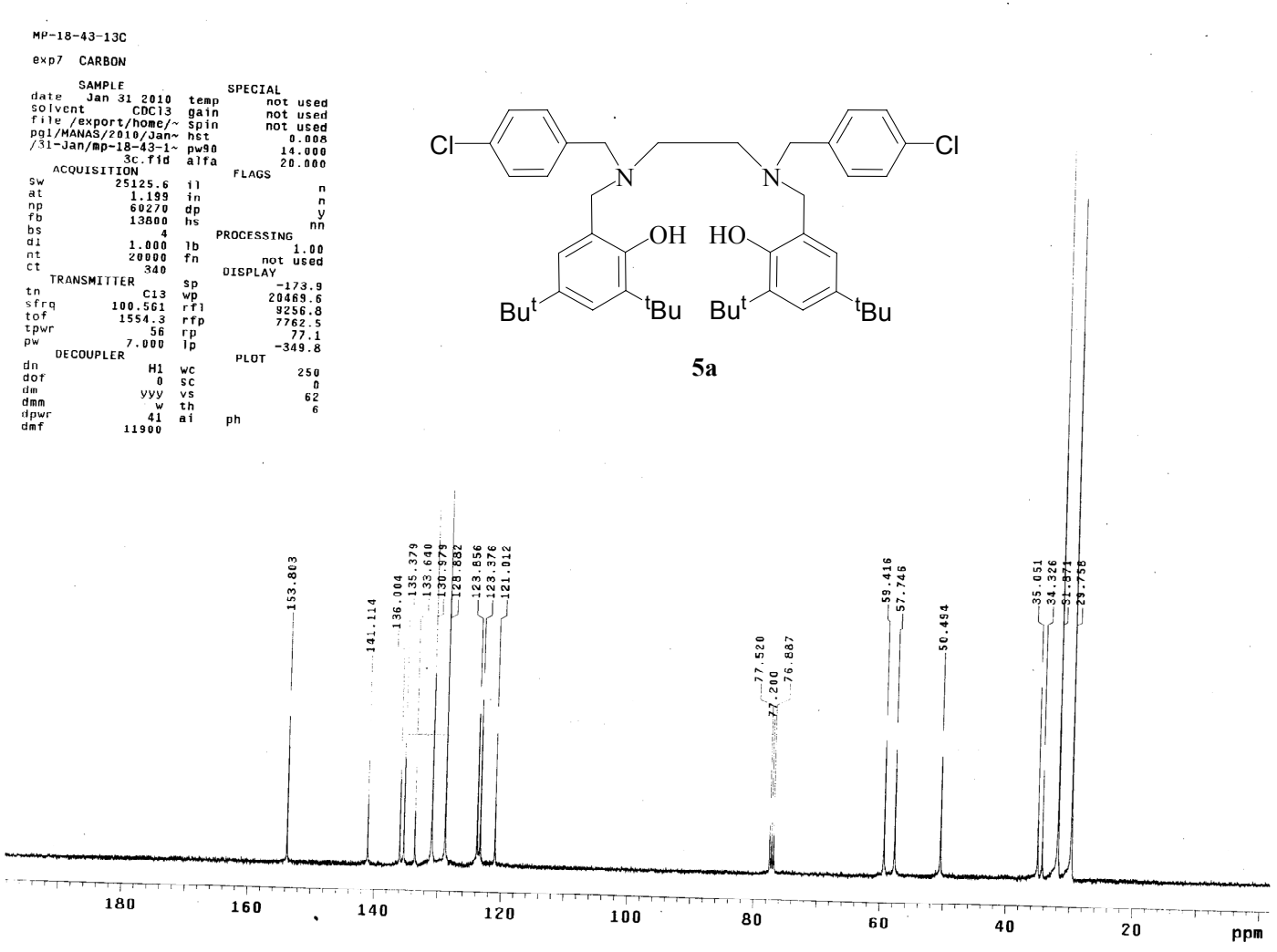


Figure S13. ^{13}C NMR spectrum of **5a** in $CDCl_3$.

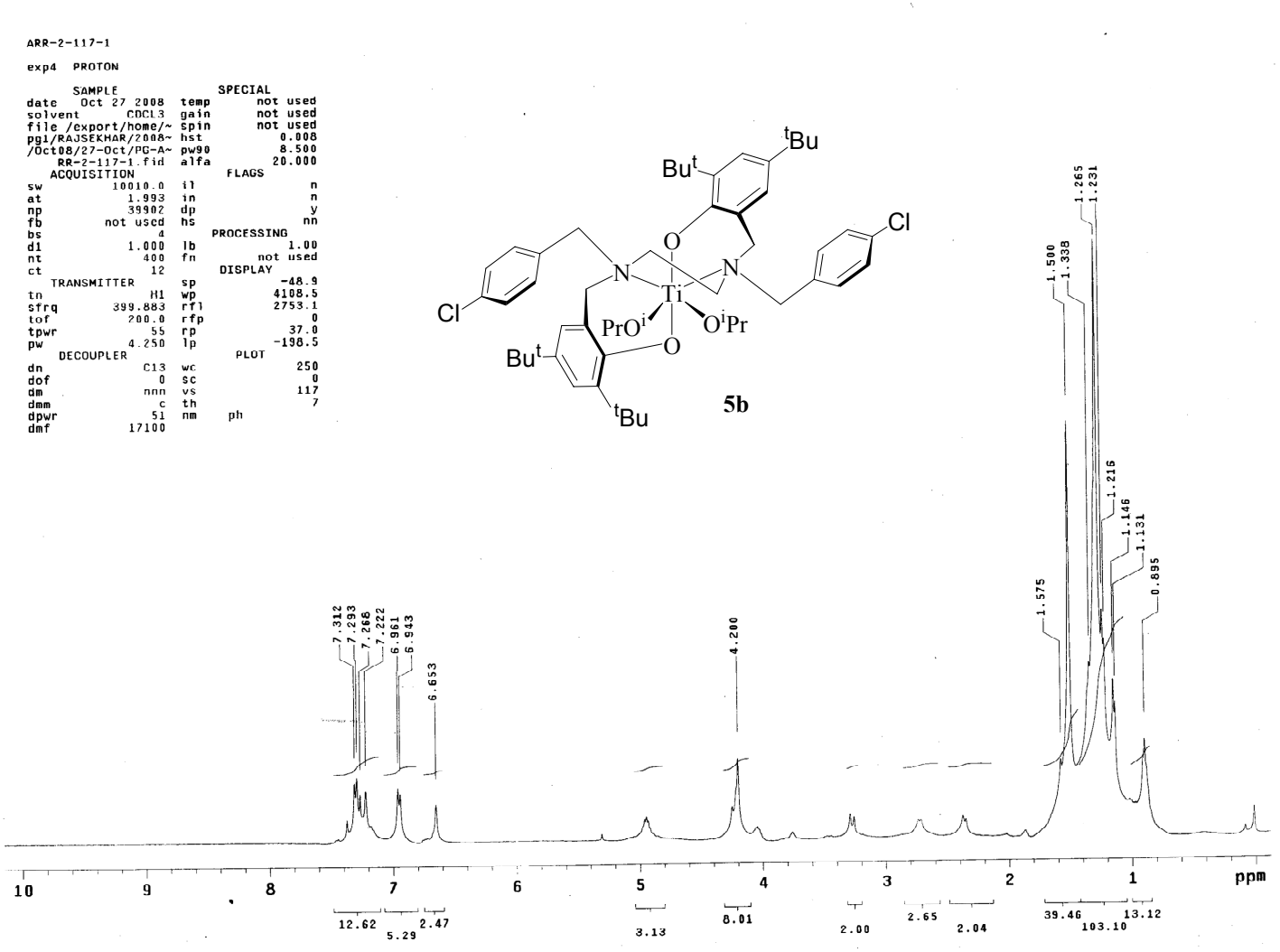


Figure S14. ^{1}H NMR spectrum of **5b** in $CDCl_3$.

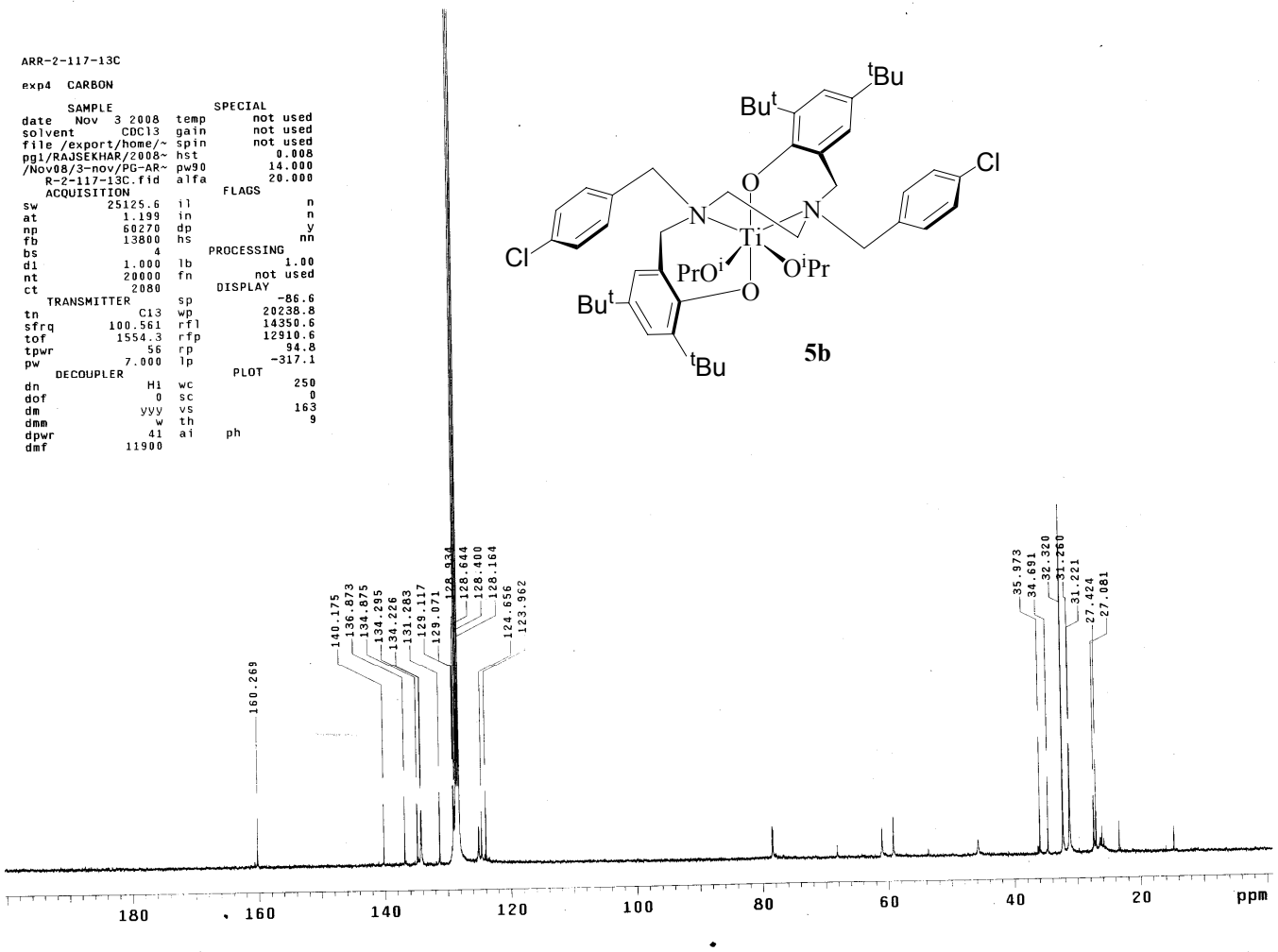


Figure S15. ^{13}C NMR spectrum of **5b** in C_6D_6.

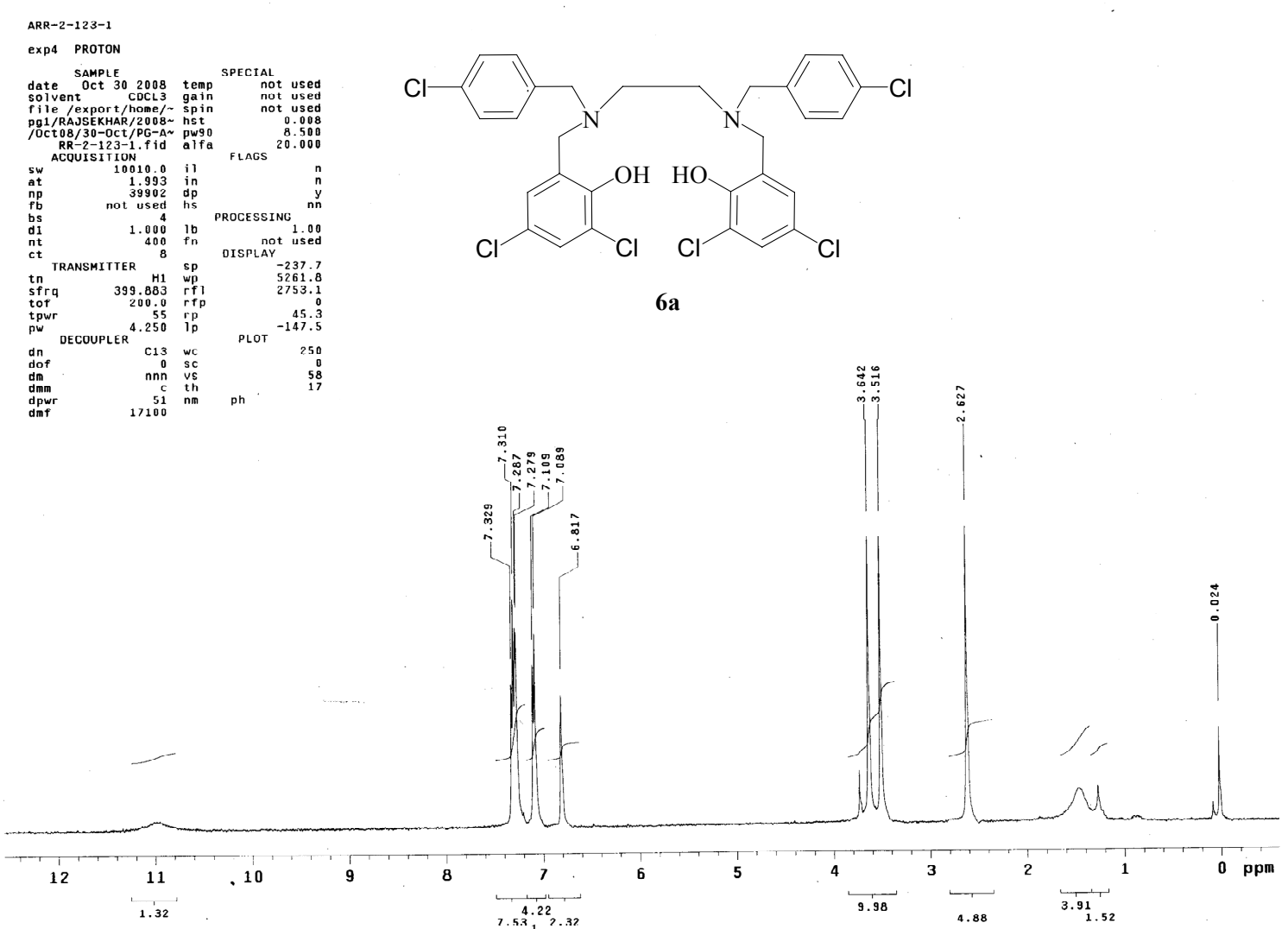


Figure S16. ^{1}H NMR spectrum of **6a** in $CDCl_3$.

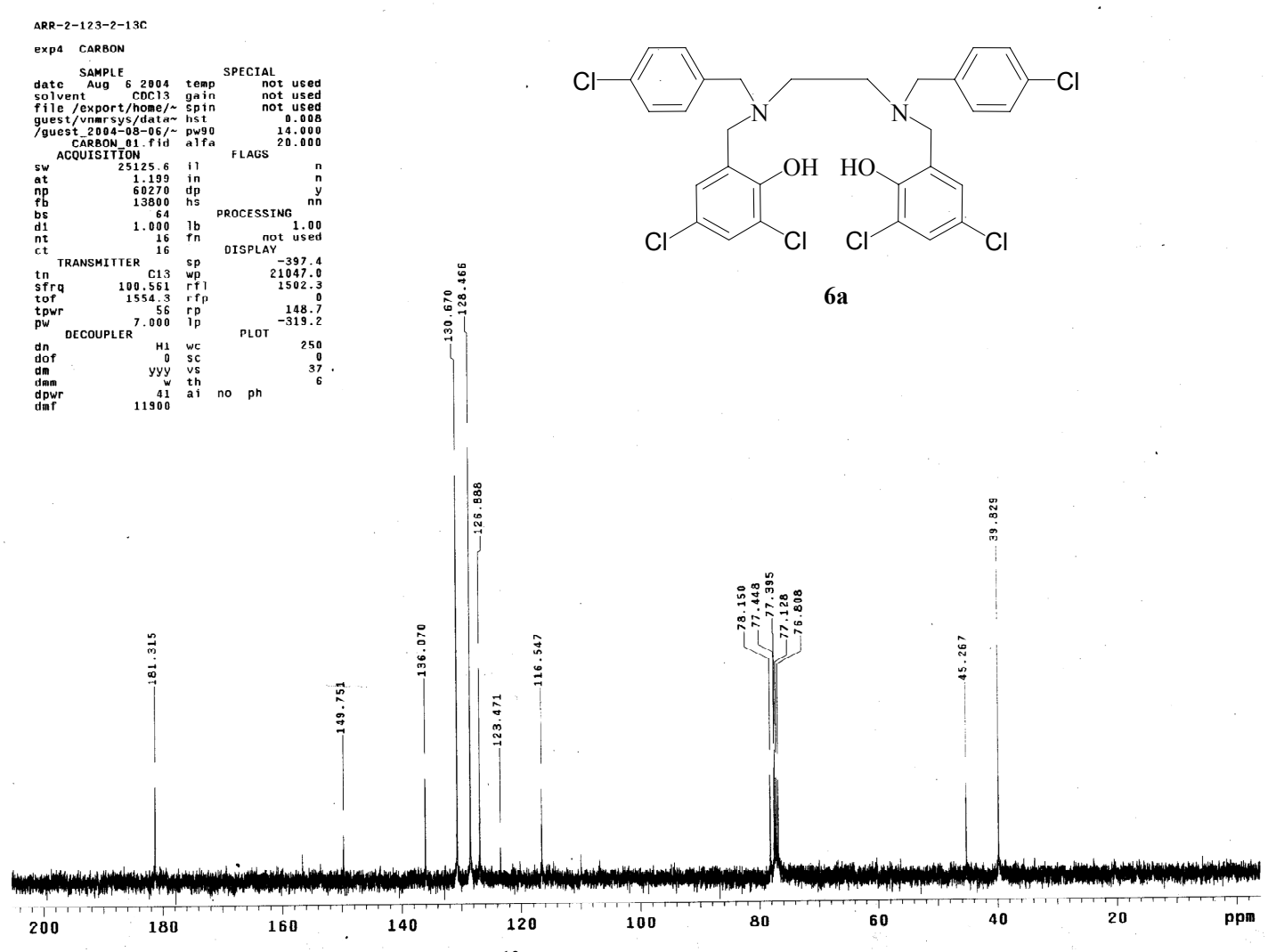


Figure S17. ^{13}C NMR spectrum of **6a** in $CDCl_3$.

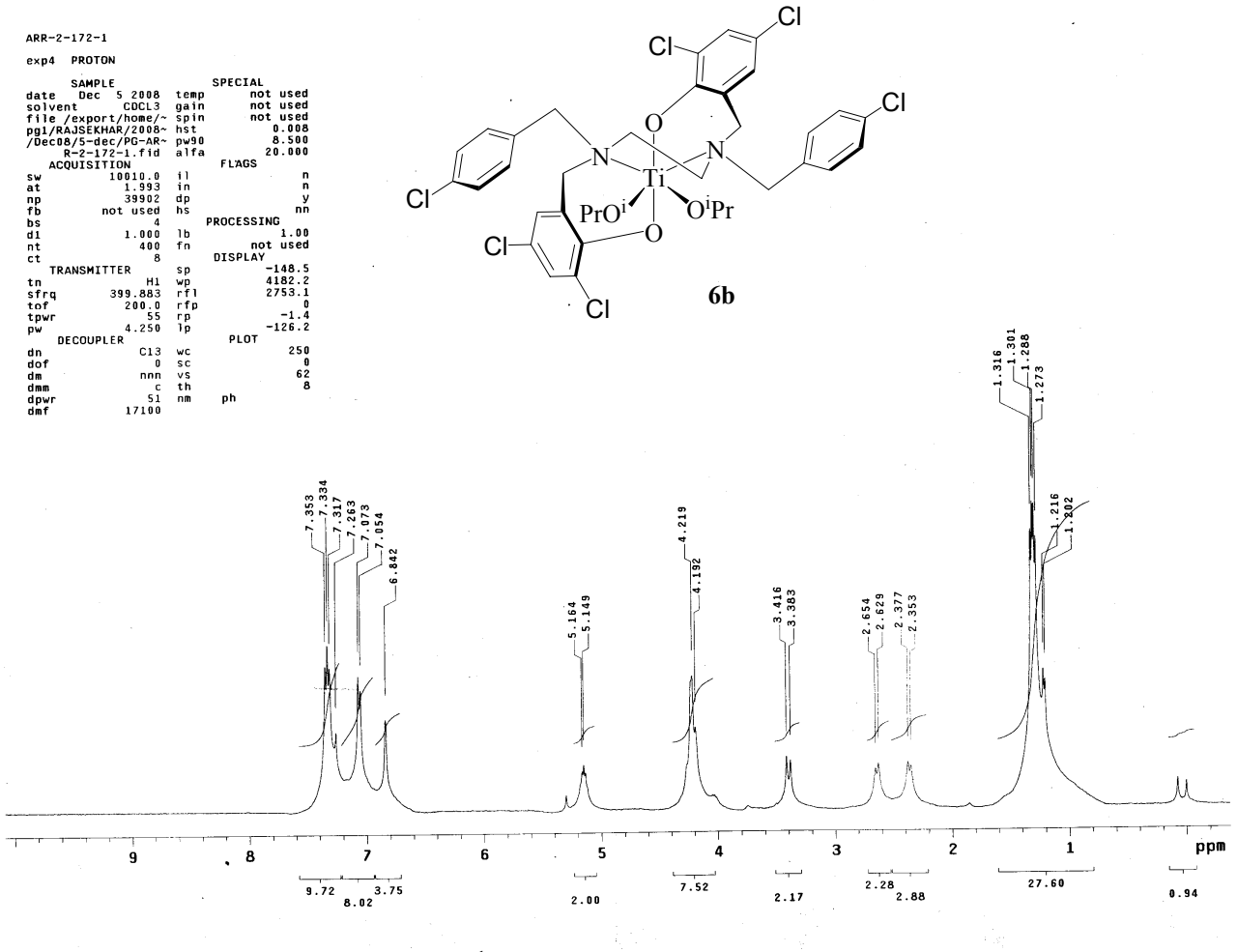


Figure S18. ^{1}H NMR spectrum of **6b** in $CDCl_3$.

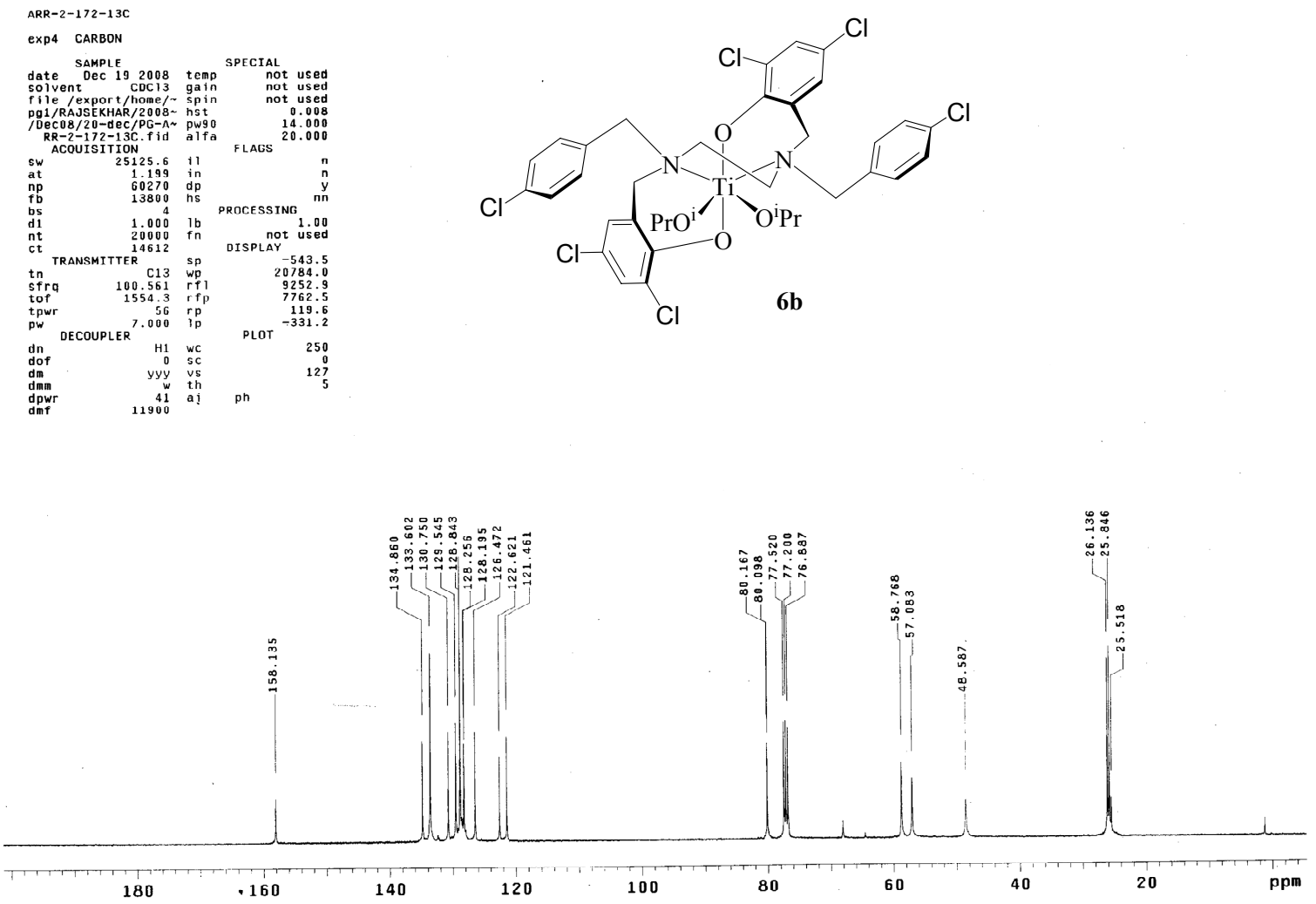


Figure S19. ^{13}C NMR spectrum of **6b** in $CDCl_3$.