

**Steric *versus* electronic factors in metallacarborane isomerisation:
nickelacarboranes with 3,1,2-, 4,1,2- and 2,1,8-NiC₂B₉ architectures and
pendant carborane groups, derived from 1,1'-bis(*o*-carborane)**

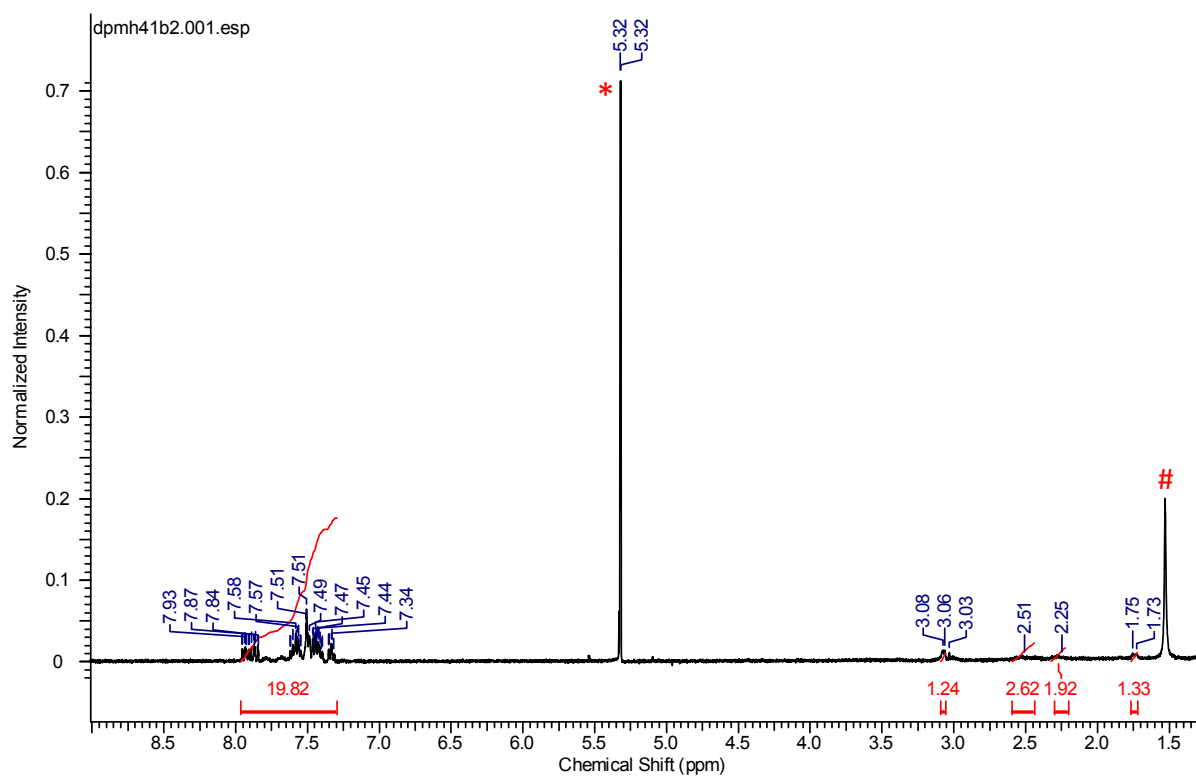
Dipendu Mandal, Wing. Y. Man, Georgina M. Rosair and Alan J. Welch

Supplementary Information

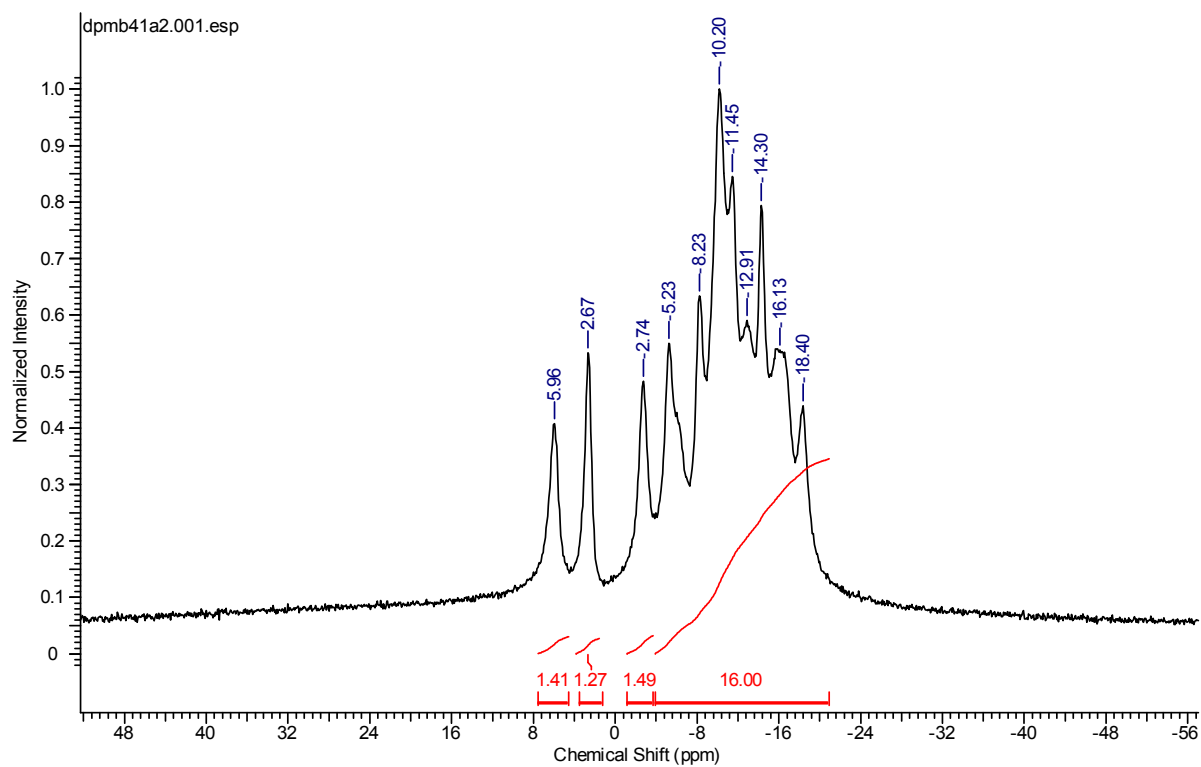
NMR spectra (¹H, ¹¹B{¹H}, ³¹P{¹H} as appropriate) for each new compound. The NMR solvents used are identified in the Experimental and references chemical shifts for residual protio solvents are CDCl₃: δ 7.27, CD₂Cl₂: δ 5.32, (CD₃)₂CO: 2.05 ppm. In the ¹H spectra solvents and water are flagged according to the following scheme: DCM, *; CHCl₃, %; (CH₃)₂CO, \$; H₂O, #

Compound **1**: [1-(1'-1',2'-*closo*-C₂B₁₀H₁₁)-3-dppe-3,1,2-*closo*-NiC₂B₉H₁₀]

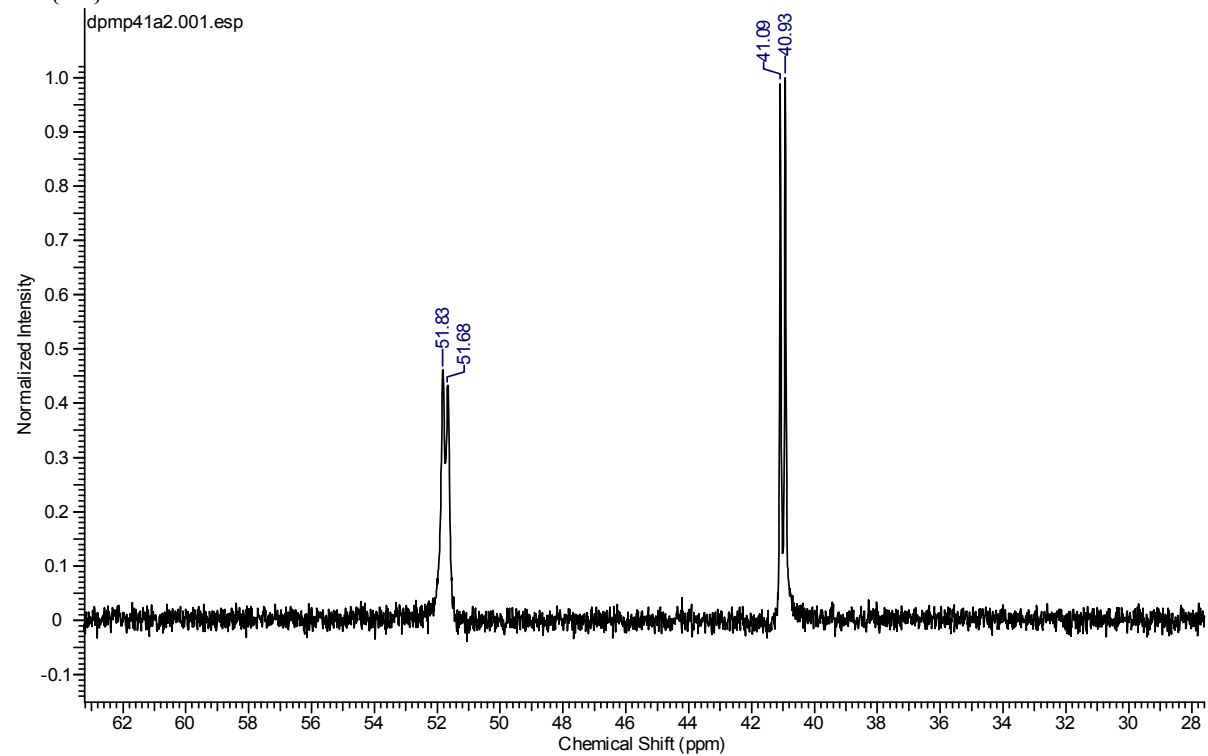
¹H NMR



¹¹B{¹H} NMR

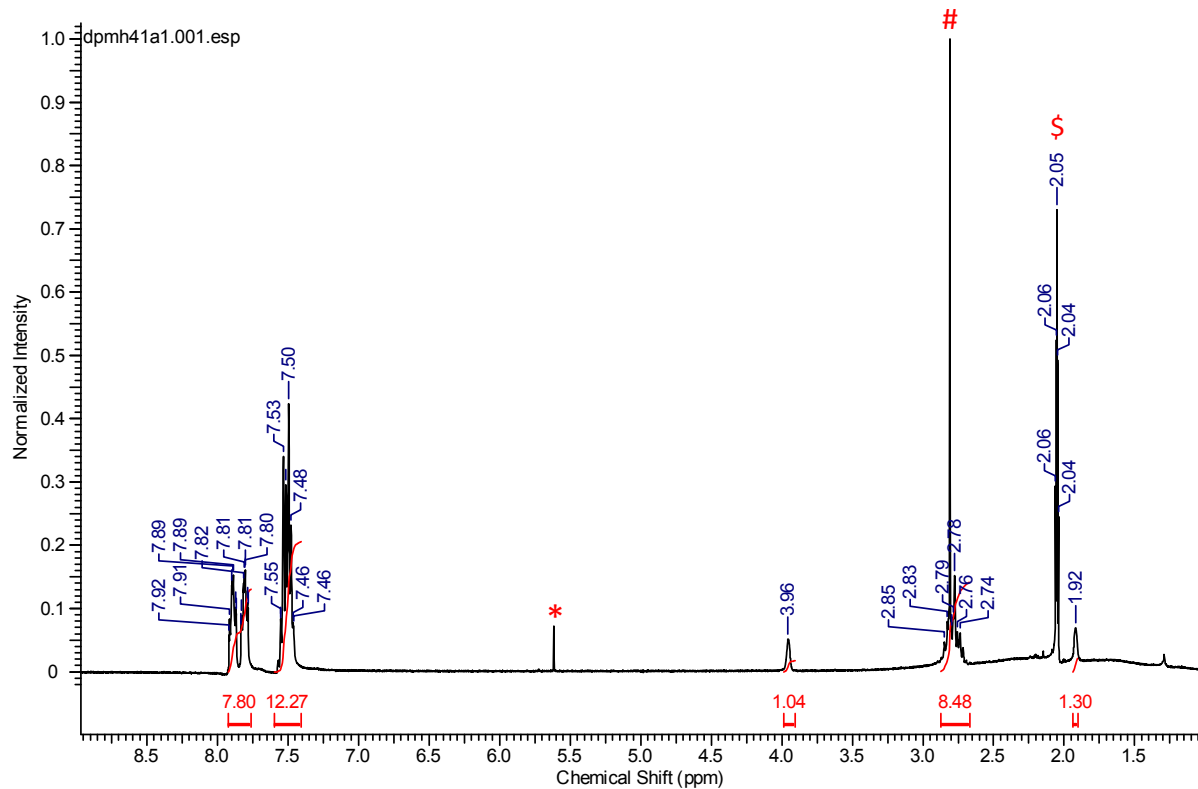


$^{31}\text{P}\{^1\text{H}\}$ NMR

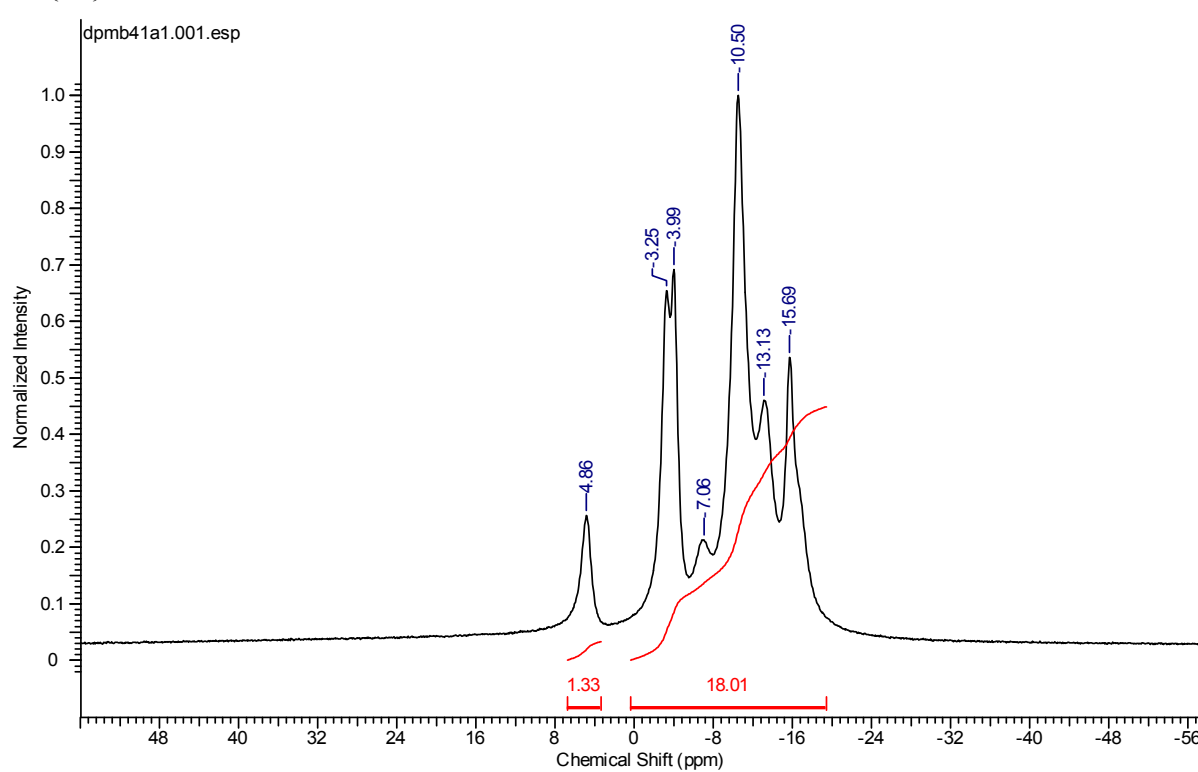


Compound 2: [2-(1'-1',2'-*closo*-C₂B₁₀H₁₁)-4-dppe-4,1,2-*closo*-NiC₂B₉H₁₀]

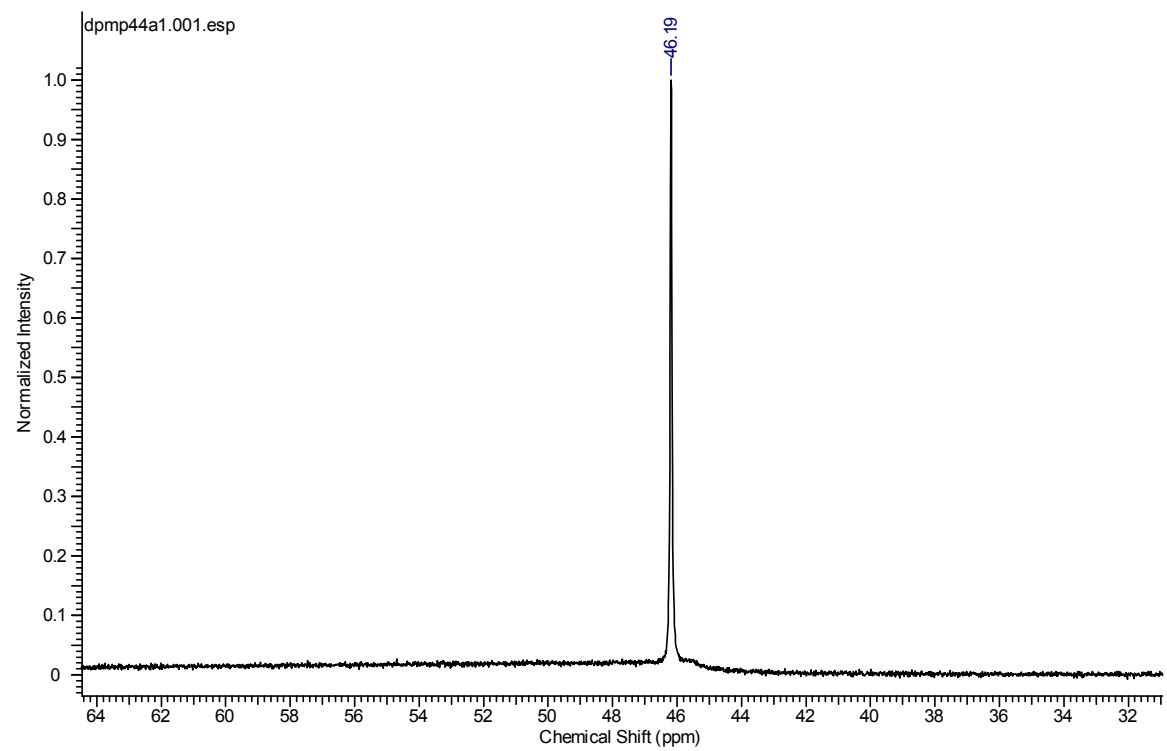
¹H NMR



¹¹B{¹H} NMR

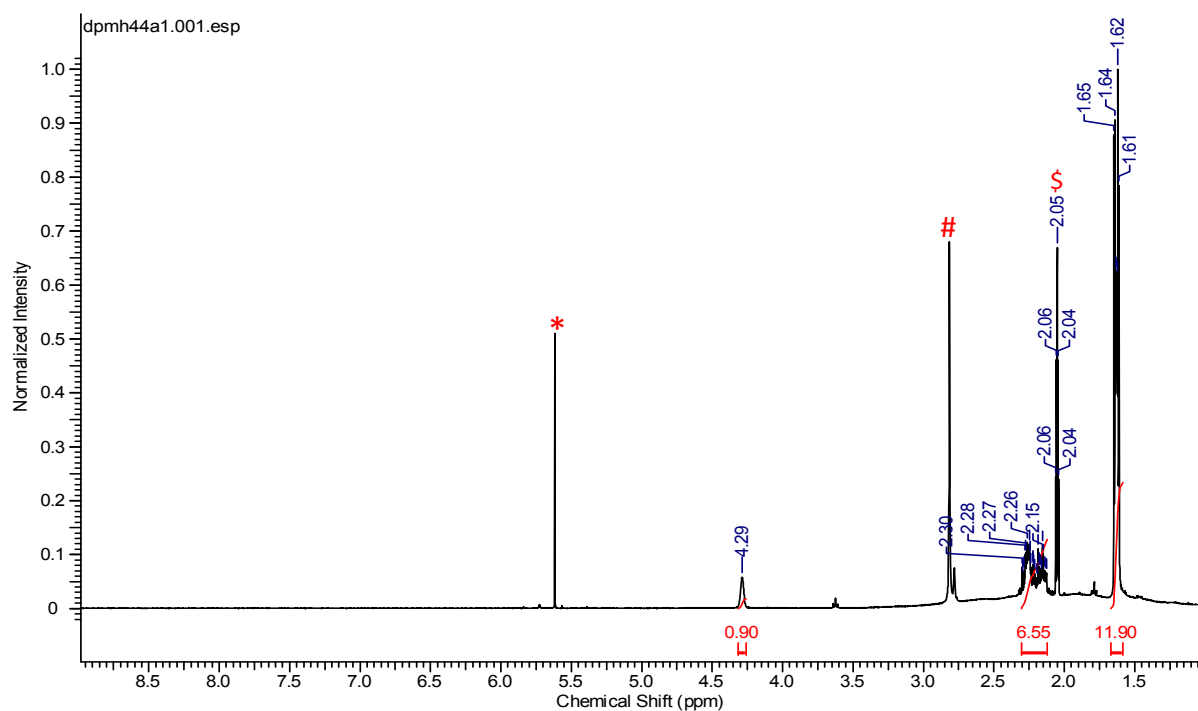


$^{31}\text{P}\{^1\text{H}\}$ NMR

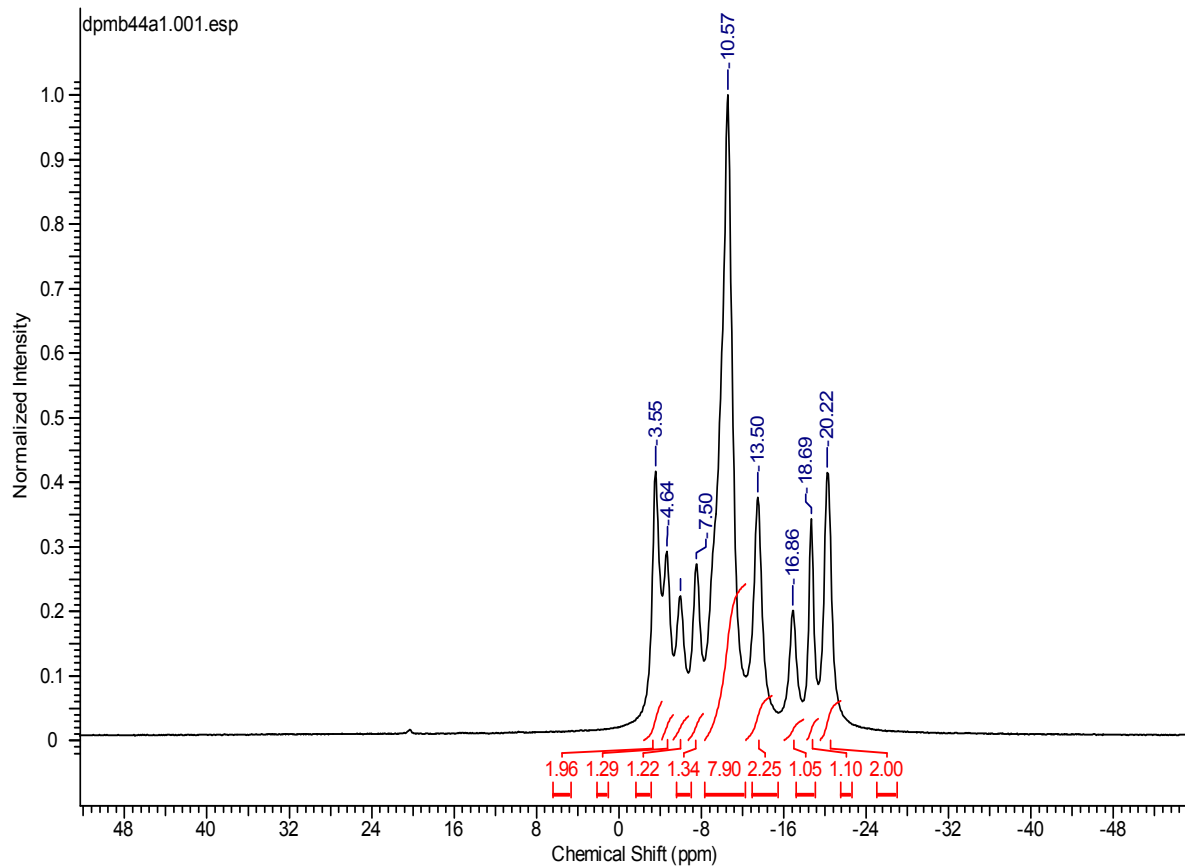


Compound **3**: [8-(1'-1',2'-*closo*-C₂B₁₀H₁₁)-2-dmpe-2,1,8-*closo*-NiC₂B₉H₁₀]

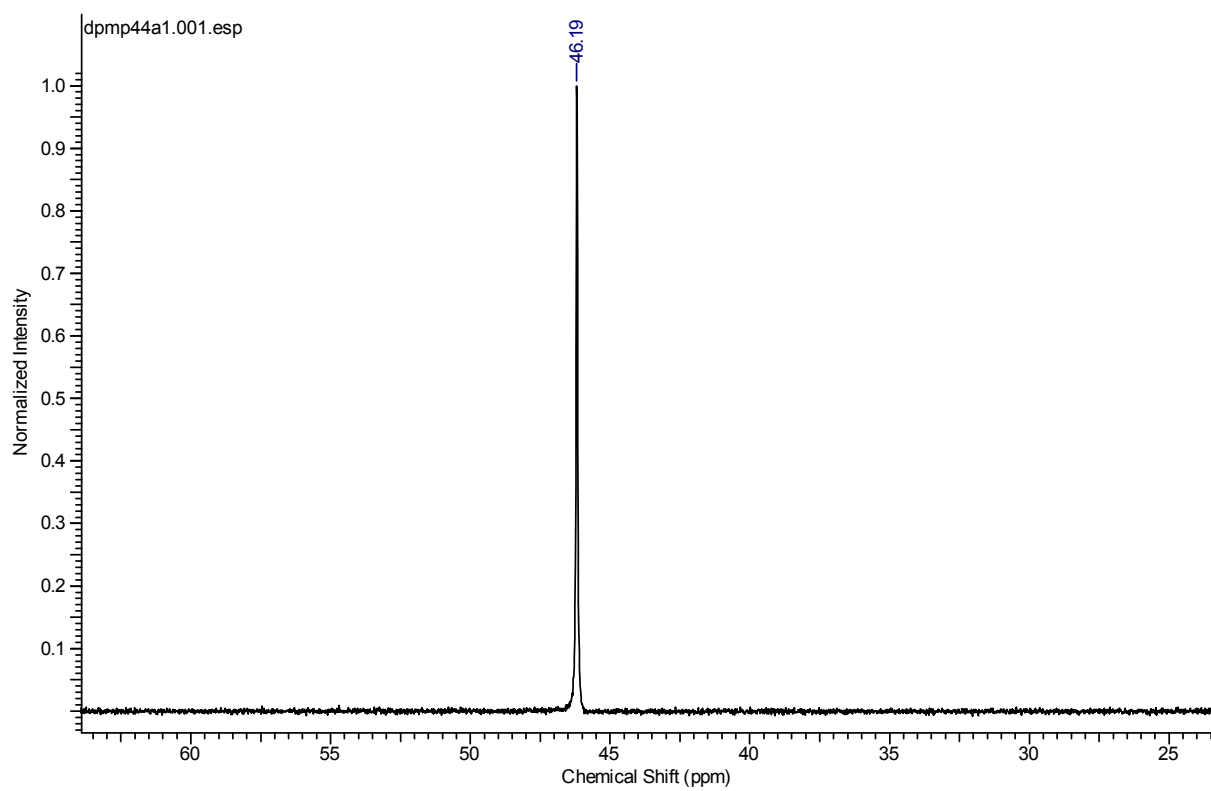
¹H NMR



¹¹B{¹H} NMR

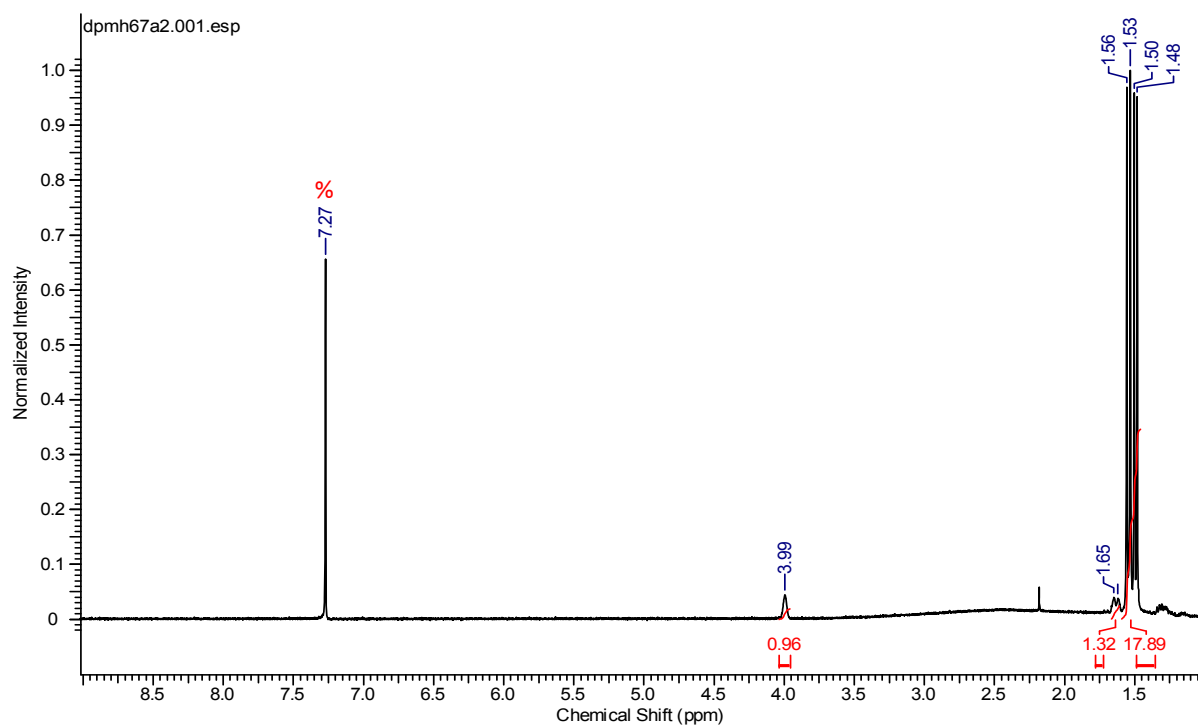


$^{31}\text{P}\{^1\text{H}\}$ NMR

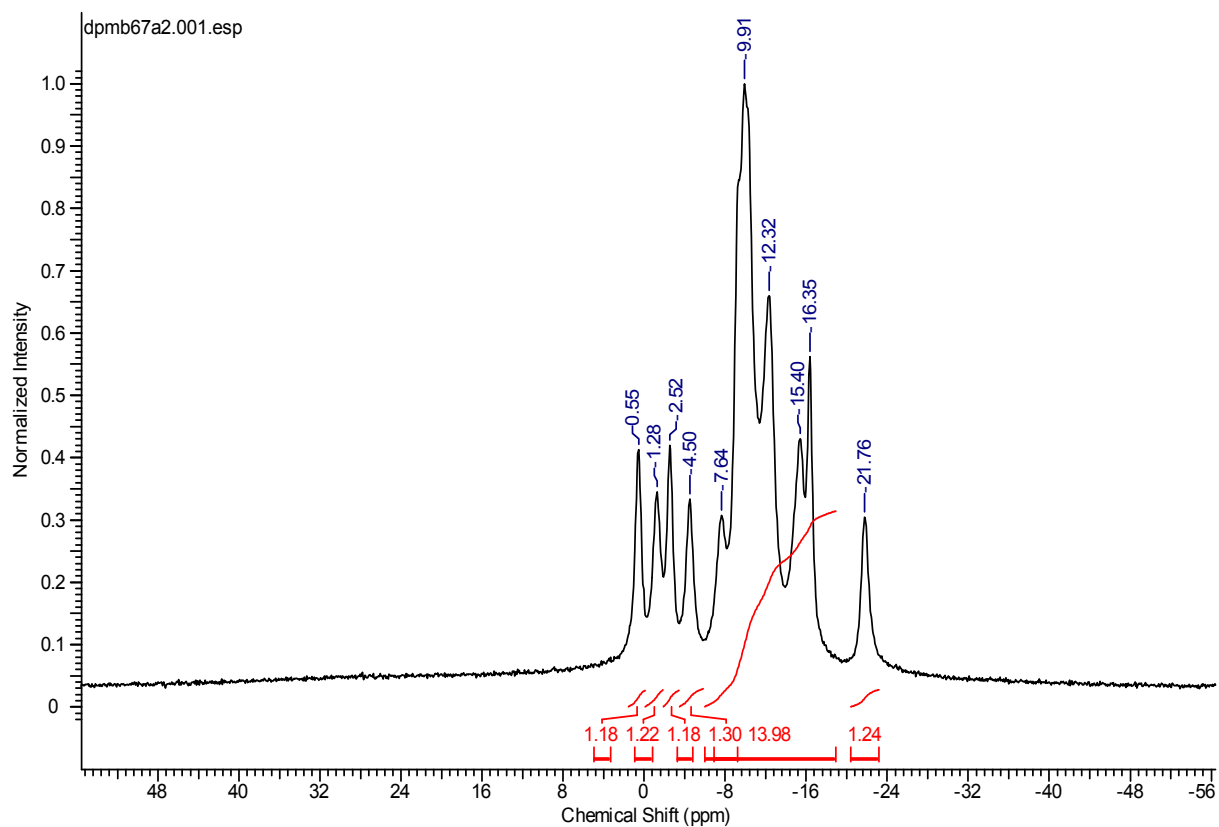


Compound 4: [1-(1'-1',2'-*closo*-C₂B₁₀H₁₁)-3,3-(PMe₃)₂-3,1,2-*closo*-NiC₂B₉H₁₀]

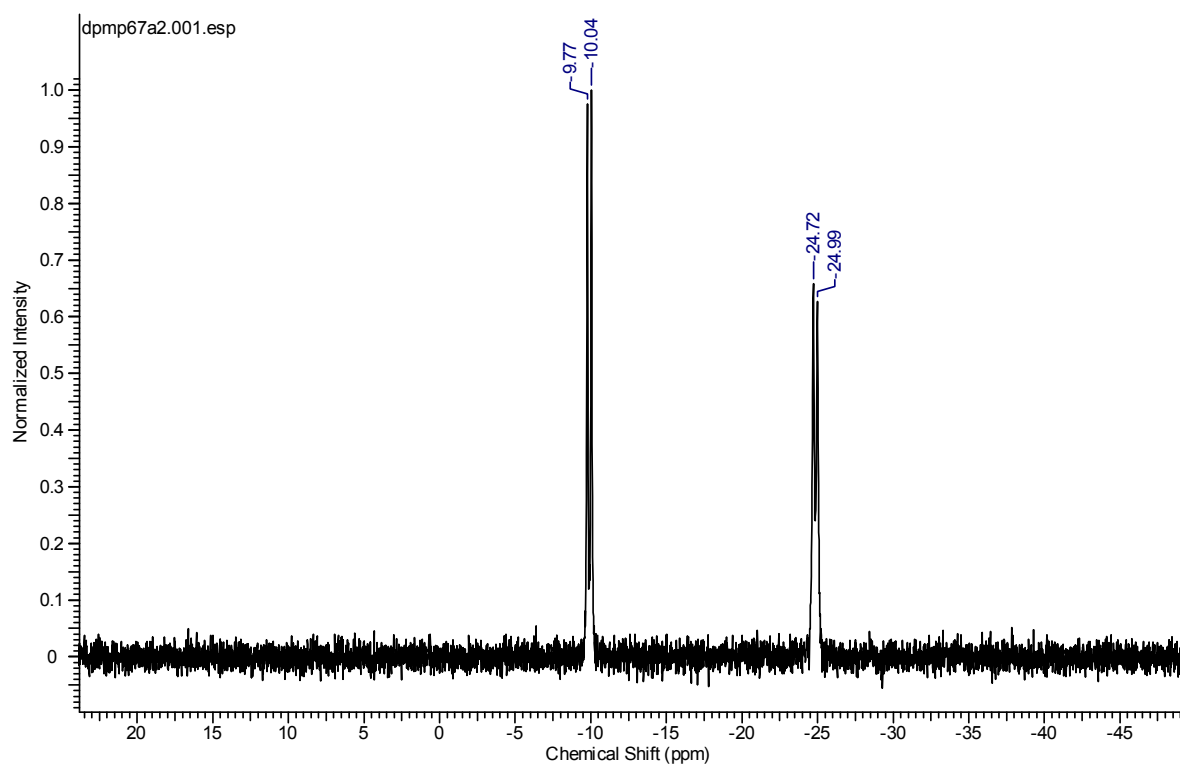
¹H NMR



¹¹B{¹H} NMR

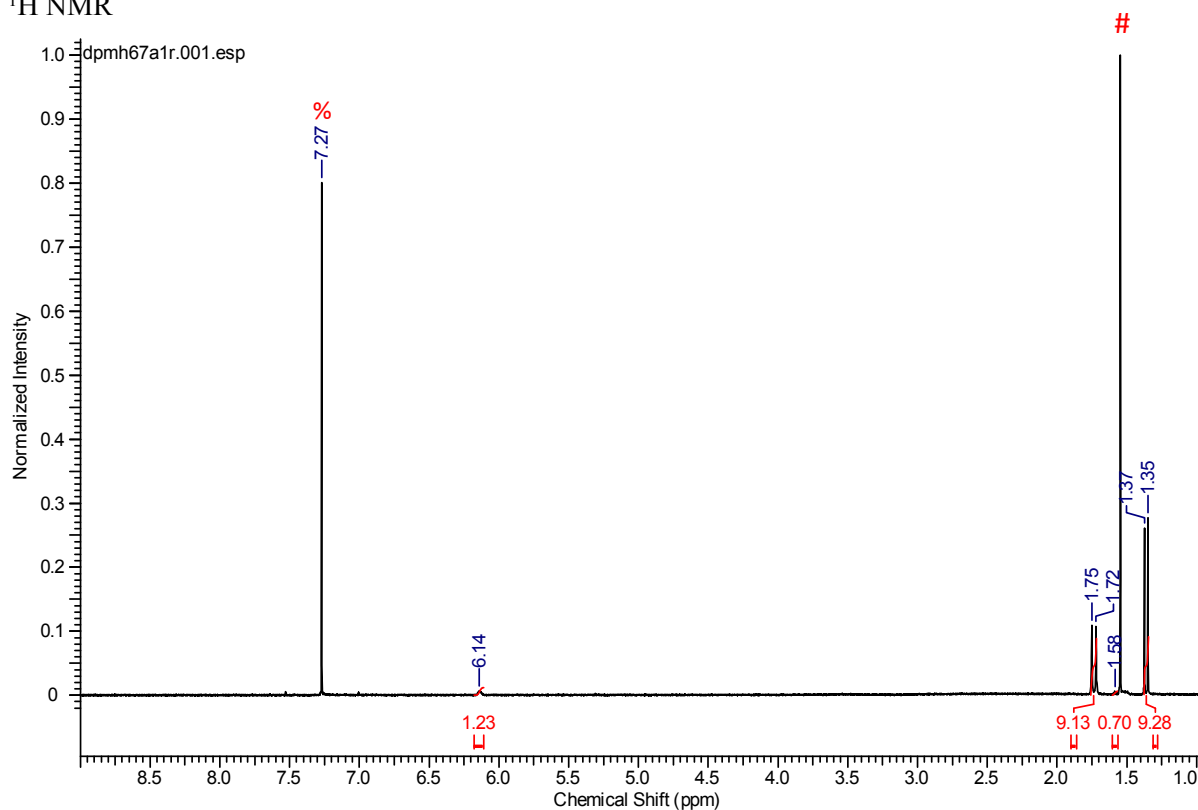


$^{31}\text{P}\{^1\text{H}\}$ NMR

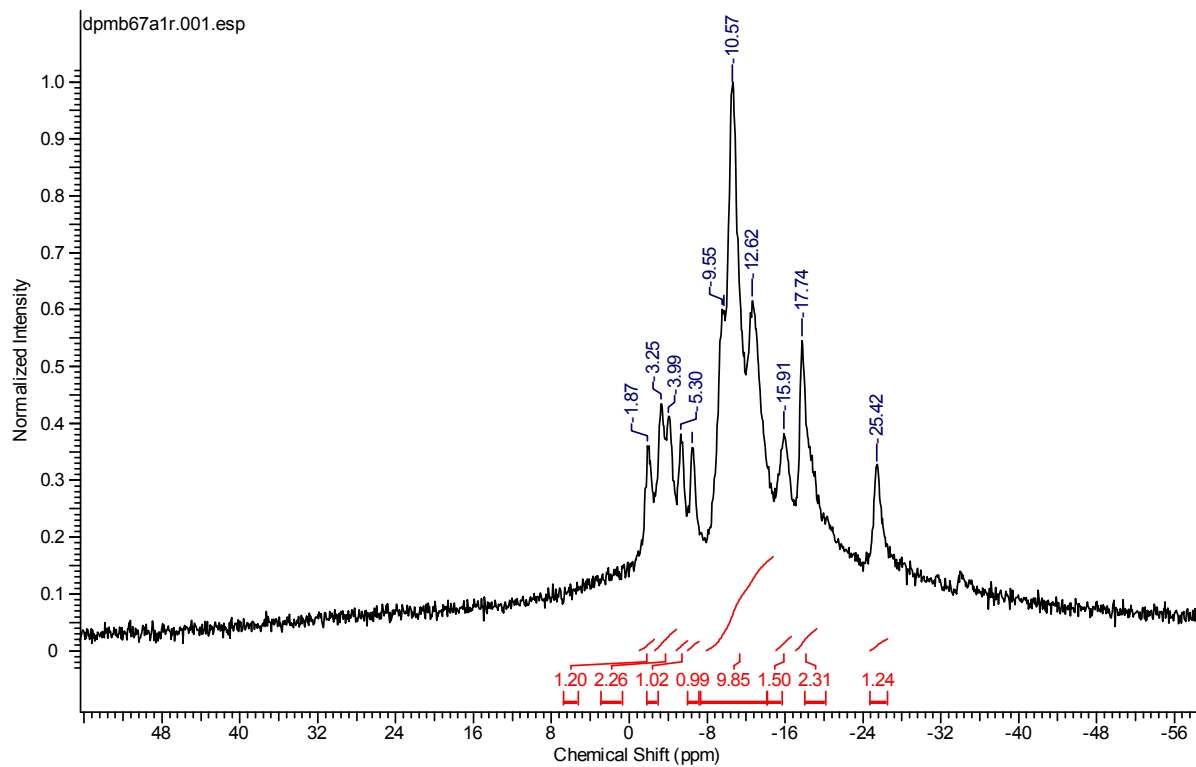


Compound **5**: [1-(1'-1',2'-*closo*-C₂B₁₀H₁₁)-3-Cl-3,8-(PMe₃)₂-3,1,2-*closo*-NiC₂B₉H₉]

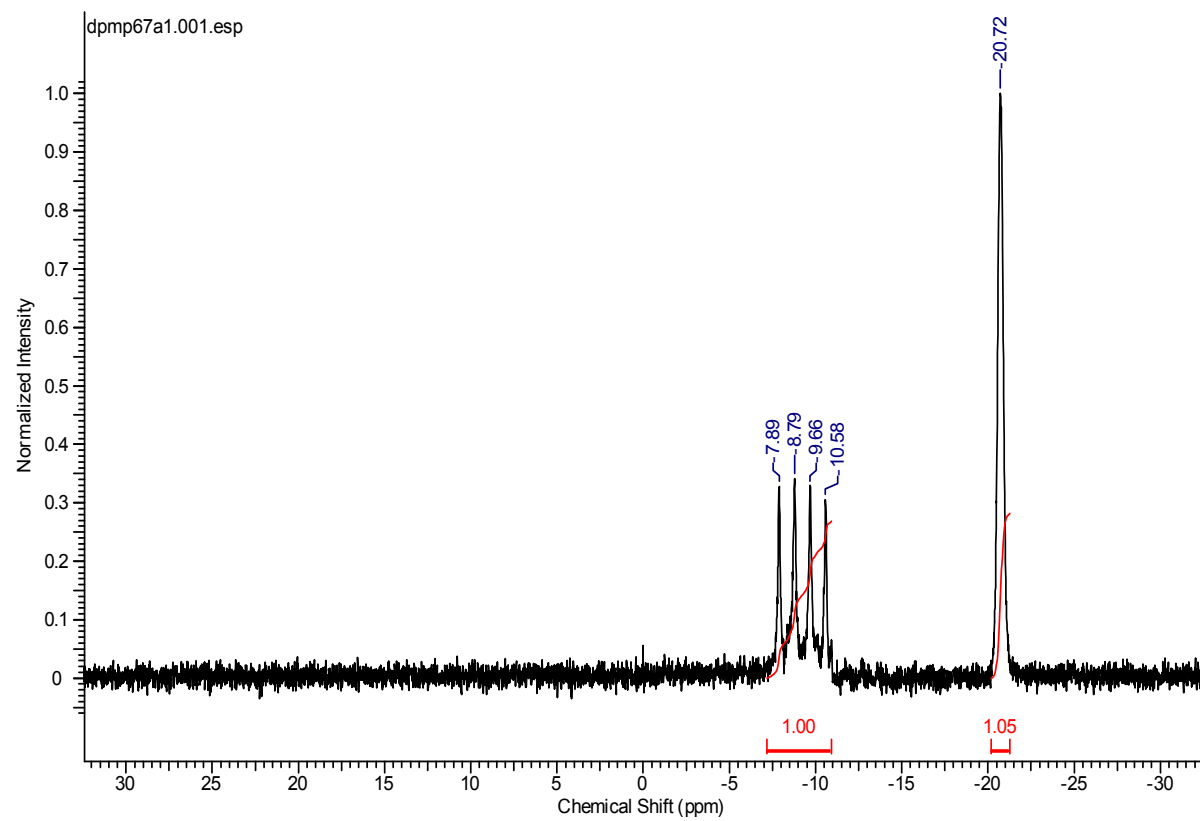
¹H NMR



¹¹B{¹H} NMR

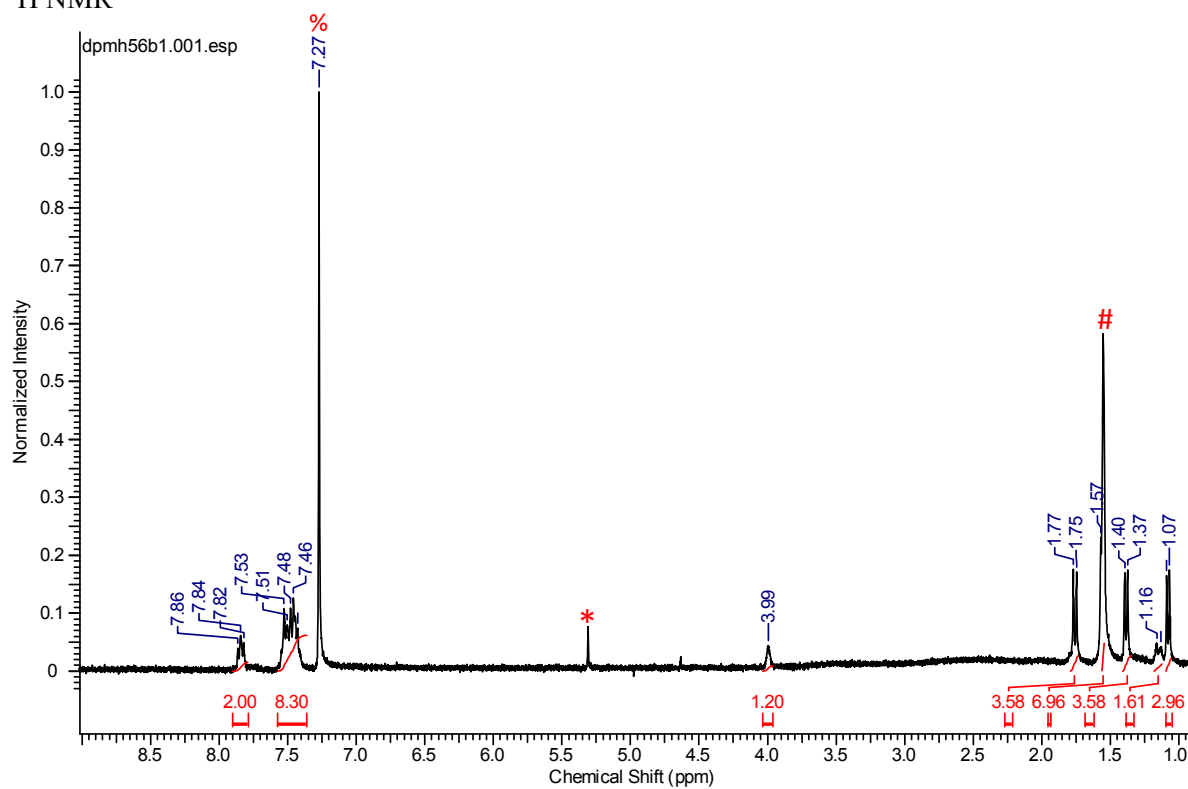


$^{31}\text{P}\{^1\text{H}\}$ NMR

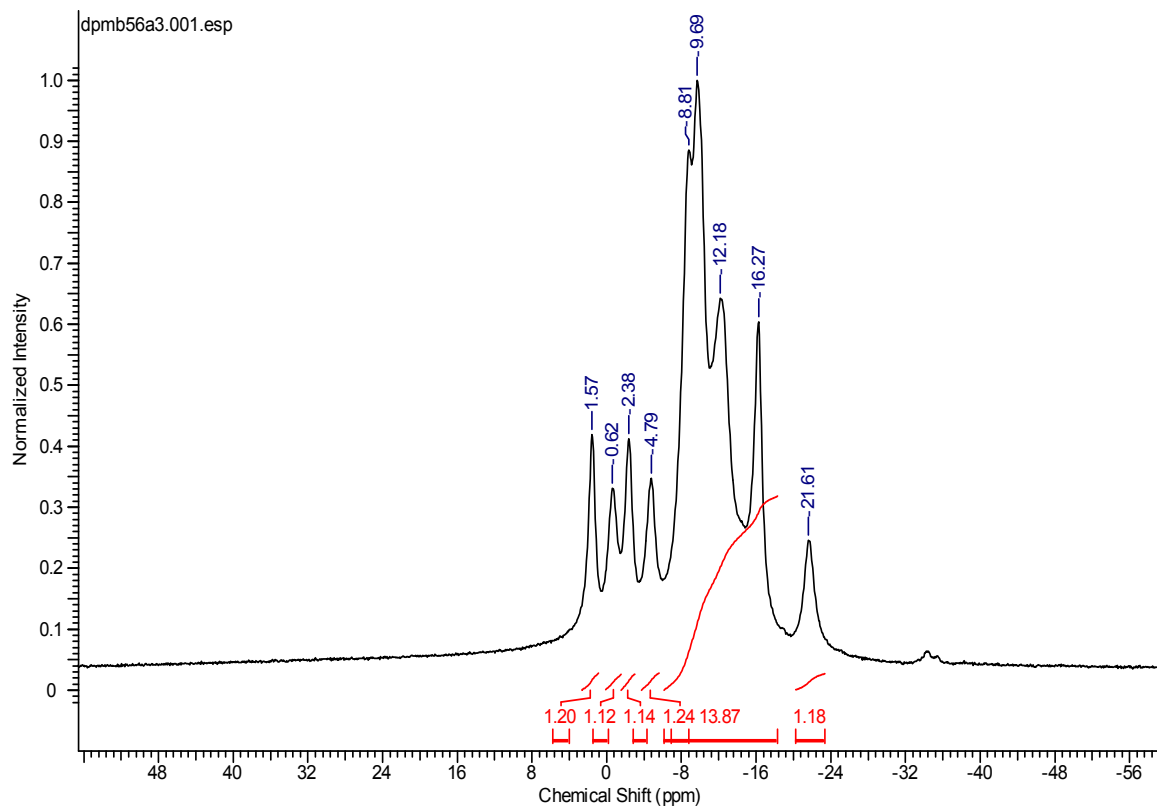


Compound 6: [1-(1'-1',2'-*closo*-C₂B₁₀H₁₁)-3,3-(PMe₂Ph)₂-3,1,2-*closo*-NiC₂B₉H₁₀]

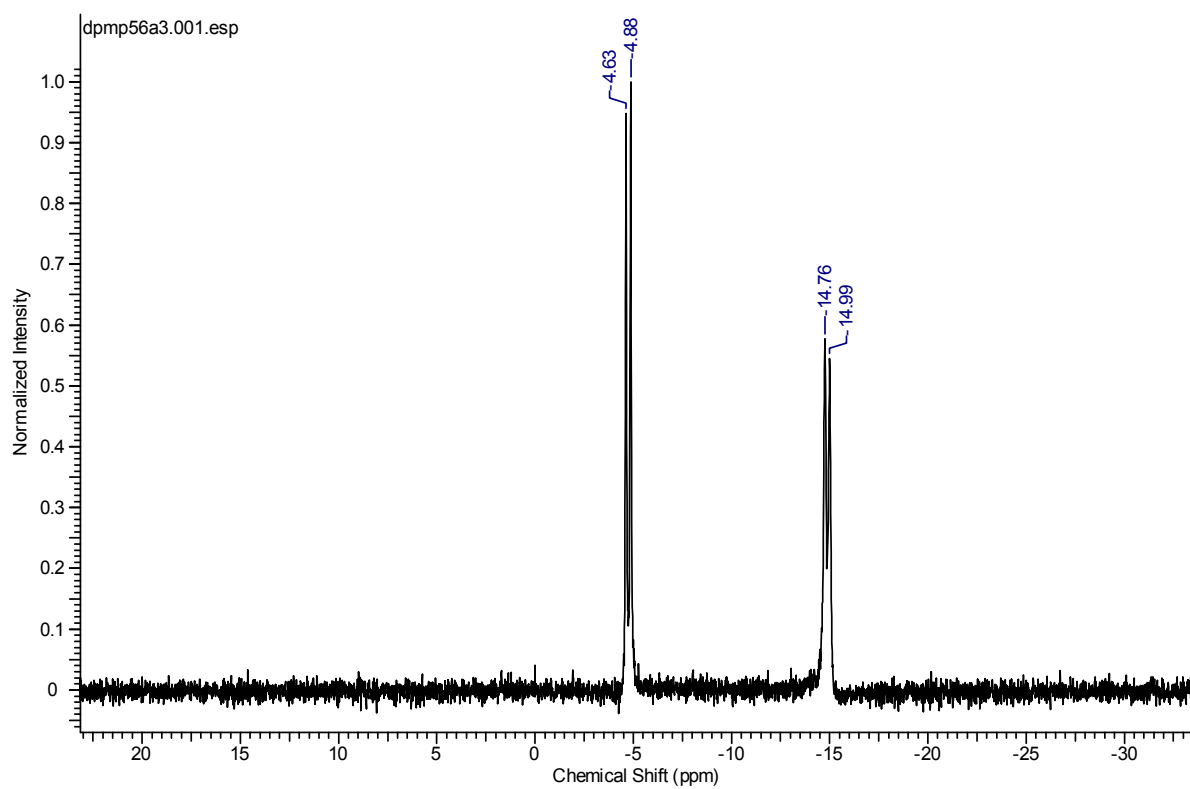
¹H NMR



¹¹B{¹H} NMR

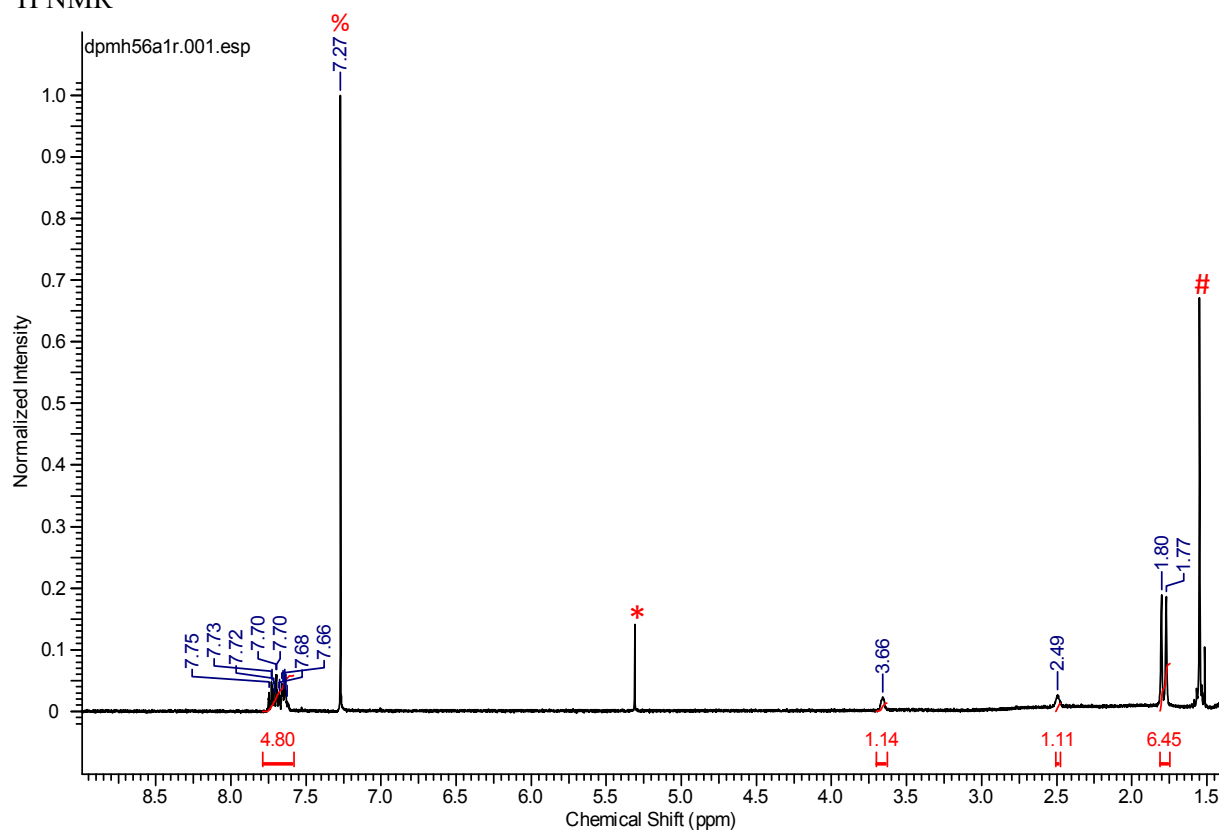


$^{31}\text{P}\{^1\text{H}\}$ NMR

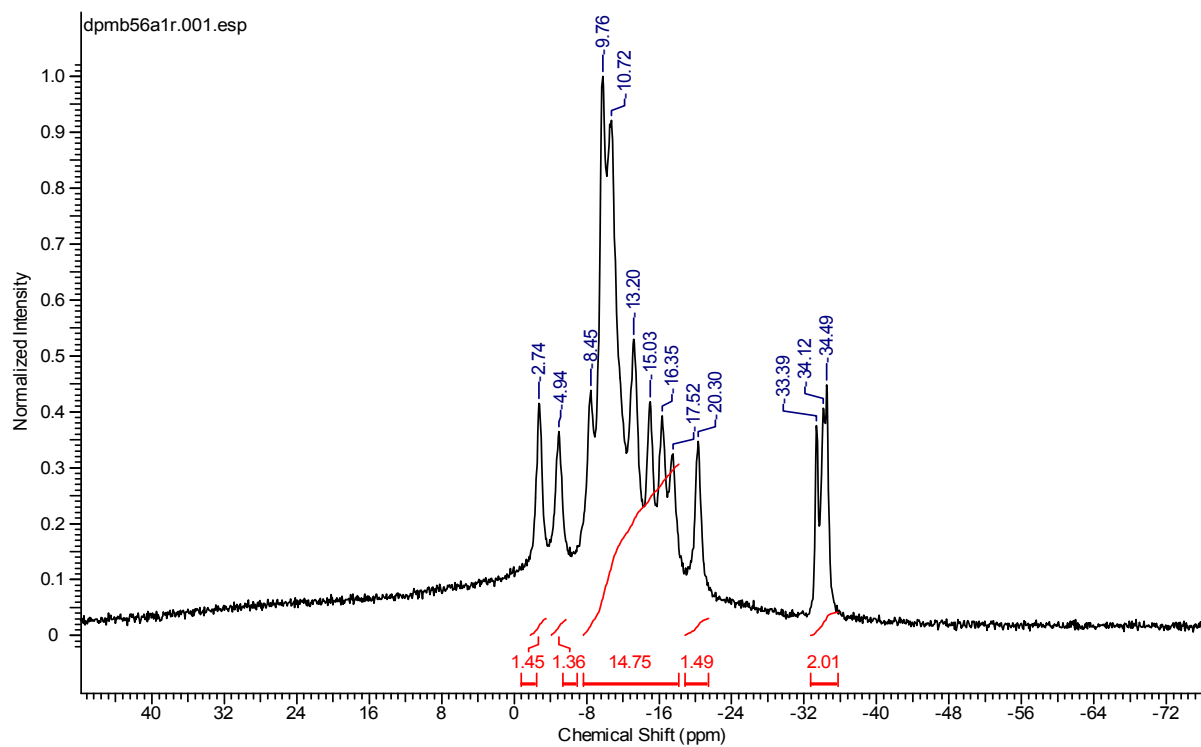


Compound 7: [7-(1'-1',2'-*closo*-C₂B₁₀H₁₁)-10-(PMe₂Ph)-7,8-*nido*-C₂B₉H₁₀]

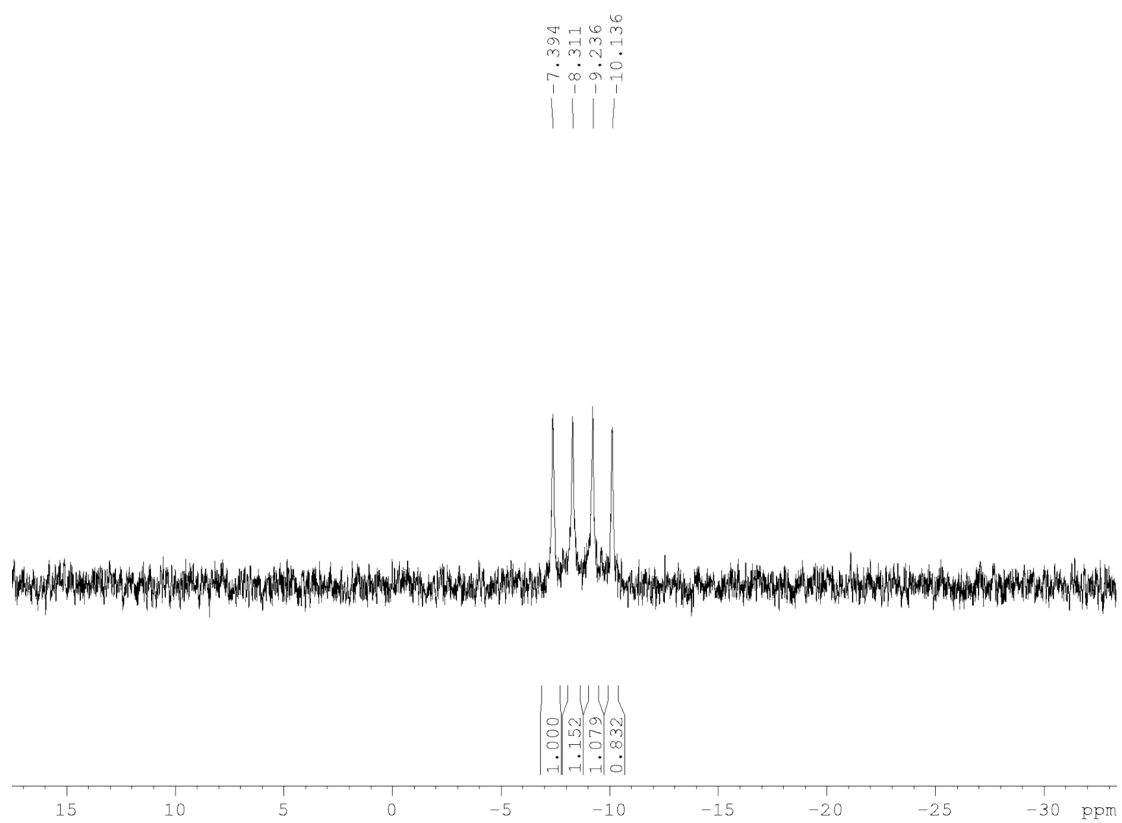
¹H NMR



¹¹B{¹H} NMR

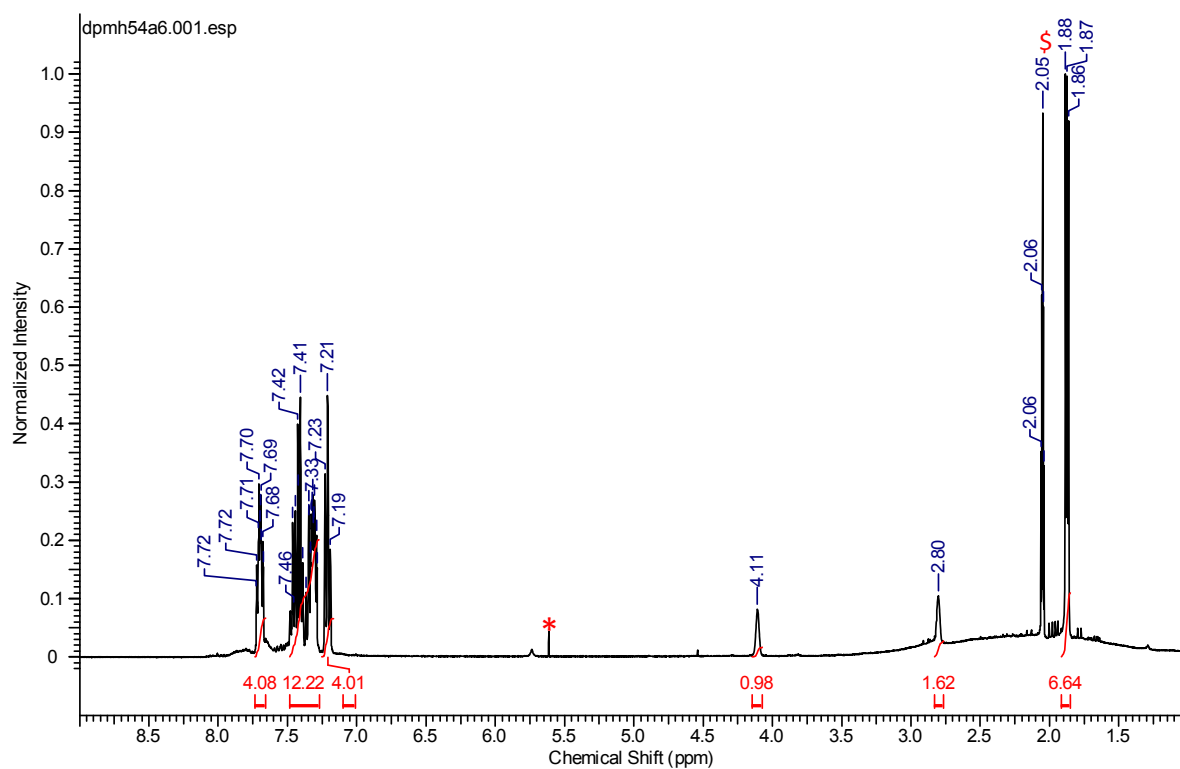


$^{31}\text{P}\{^1\text{H}\}$ NMR

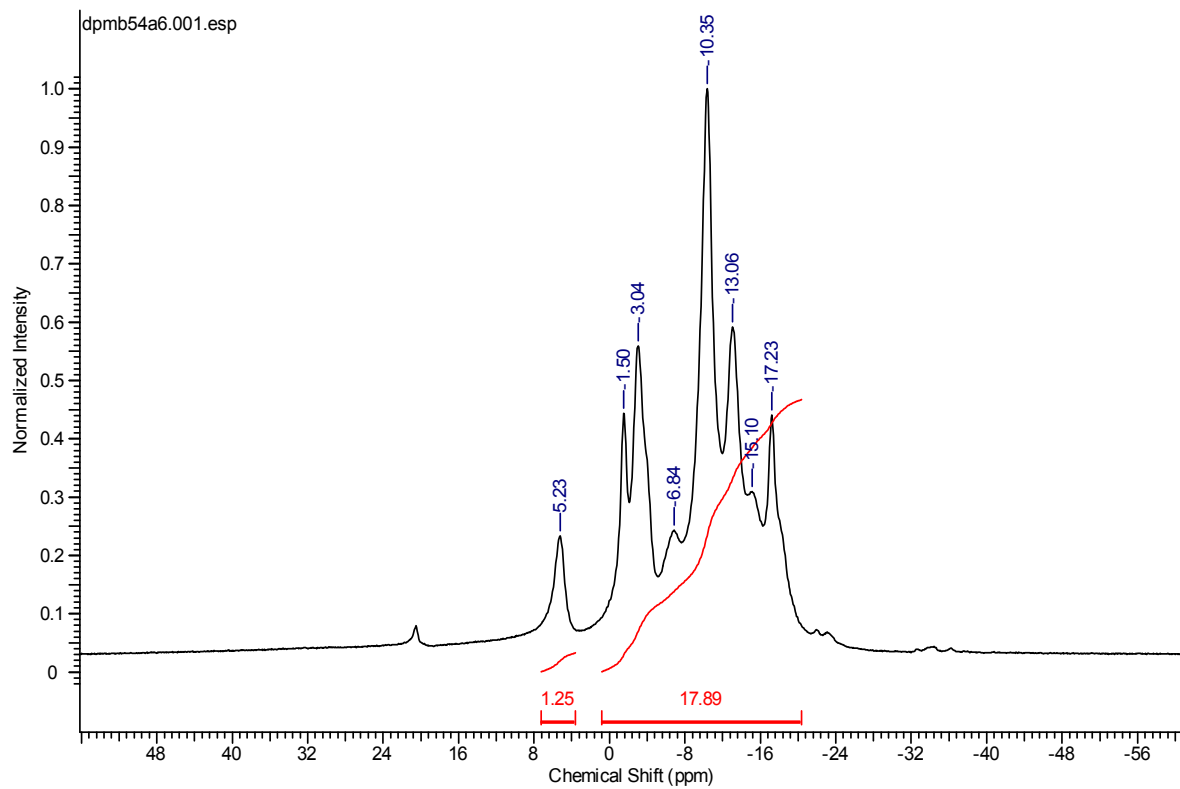


Compound **8**: [2-(1'-1',2'-*closo*-C₂B₁₀H₁₁)-4,4-(PMePh₂)₂-4,1,2-*closo*-NiC₂B₉H₁₀]

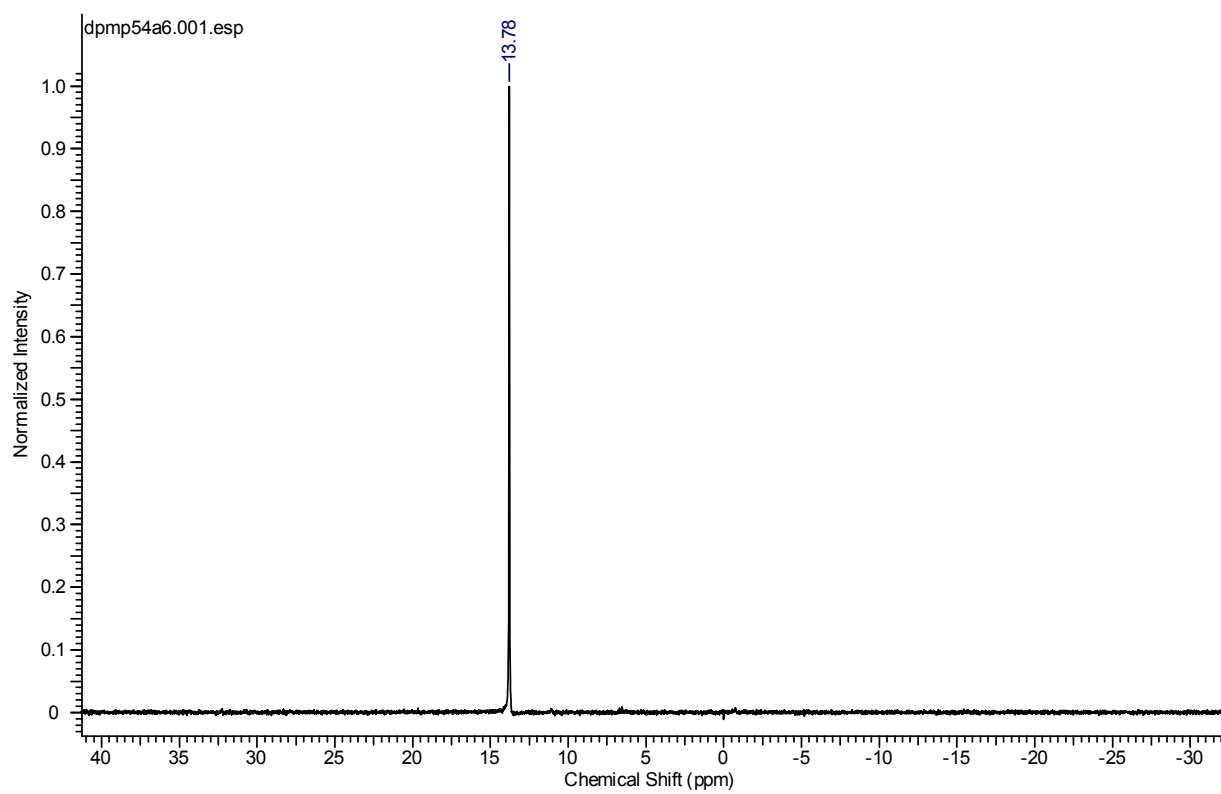
¹H NMR



¹¹B{¹H} NMR

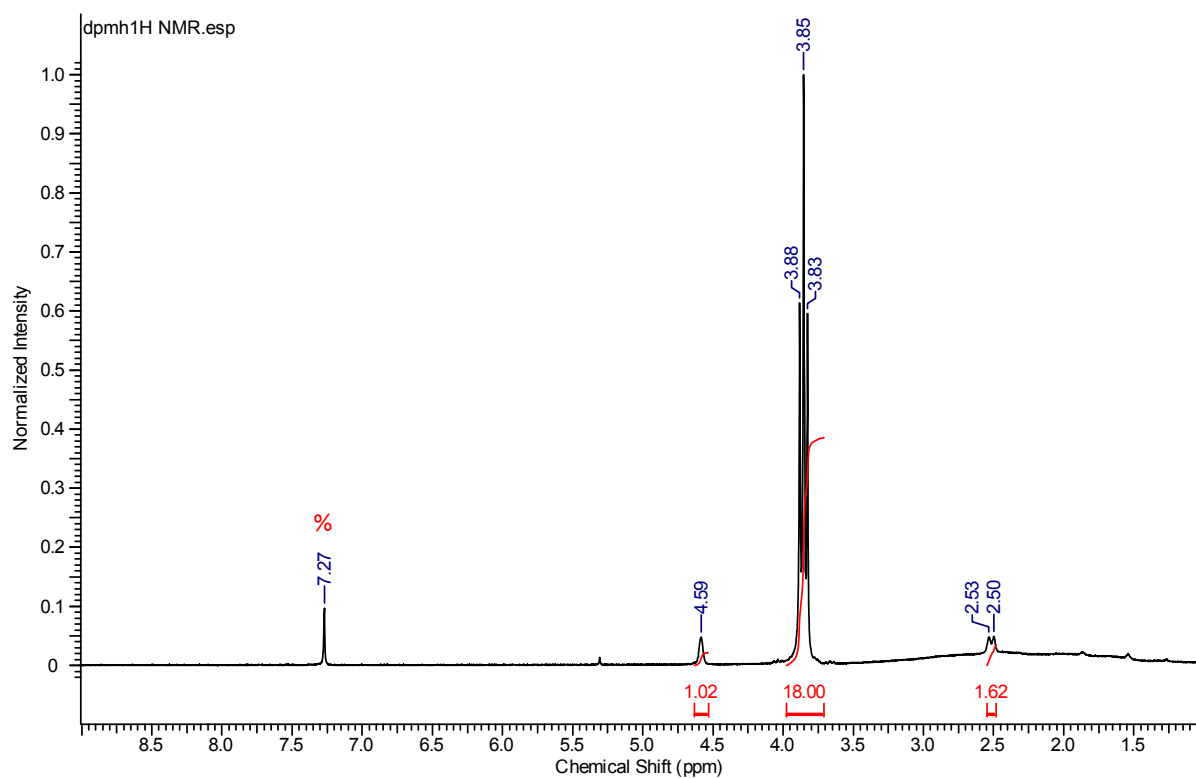


$^{31}\text{P}\{^1\text{H}\}$ NMR

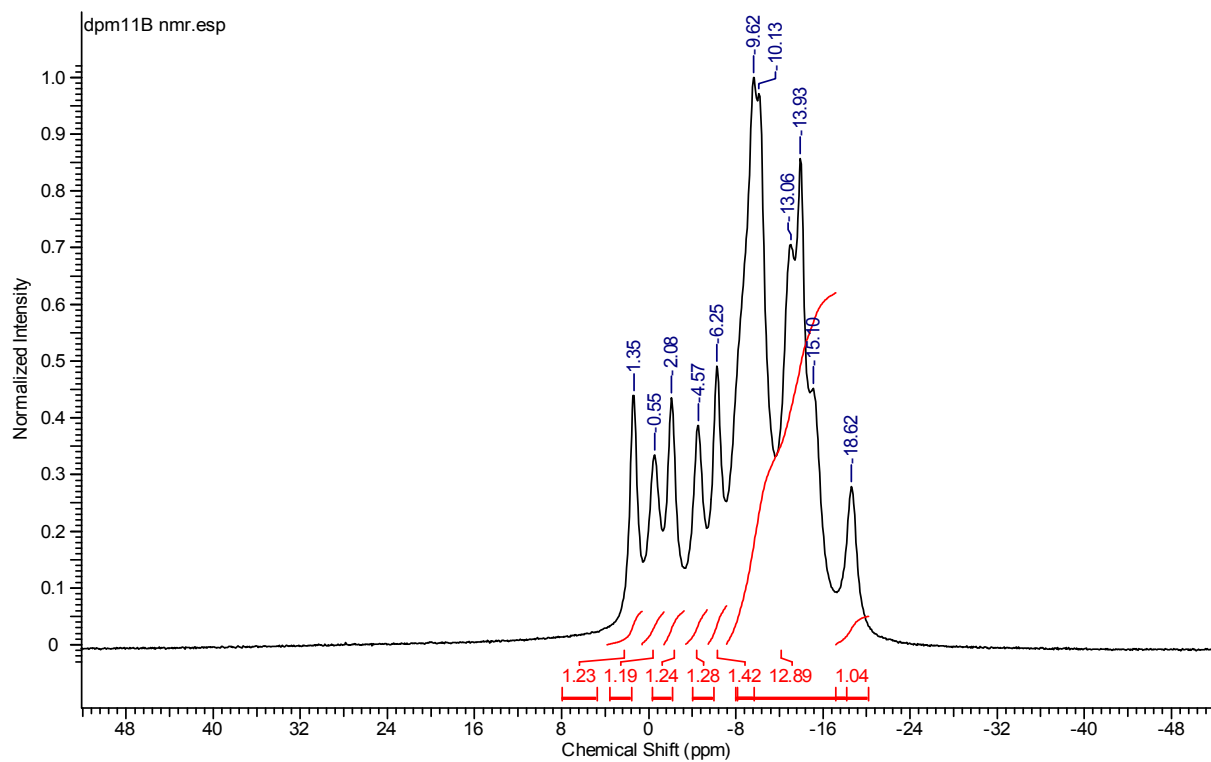


Compound **9**: [1-(1'-1',2'-*closo*-C₂B₁₀H₁₁)-3,3-{P(OMe)₃}₂-3,1,2-*closo*-NiC₂B₉H₁₀]

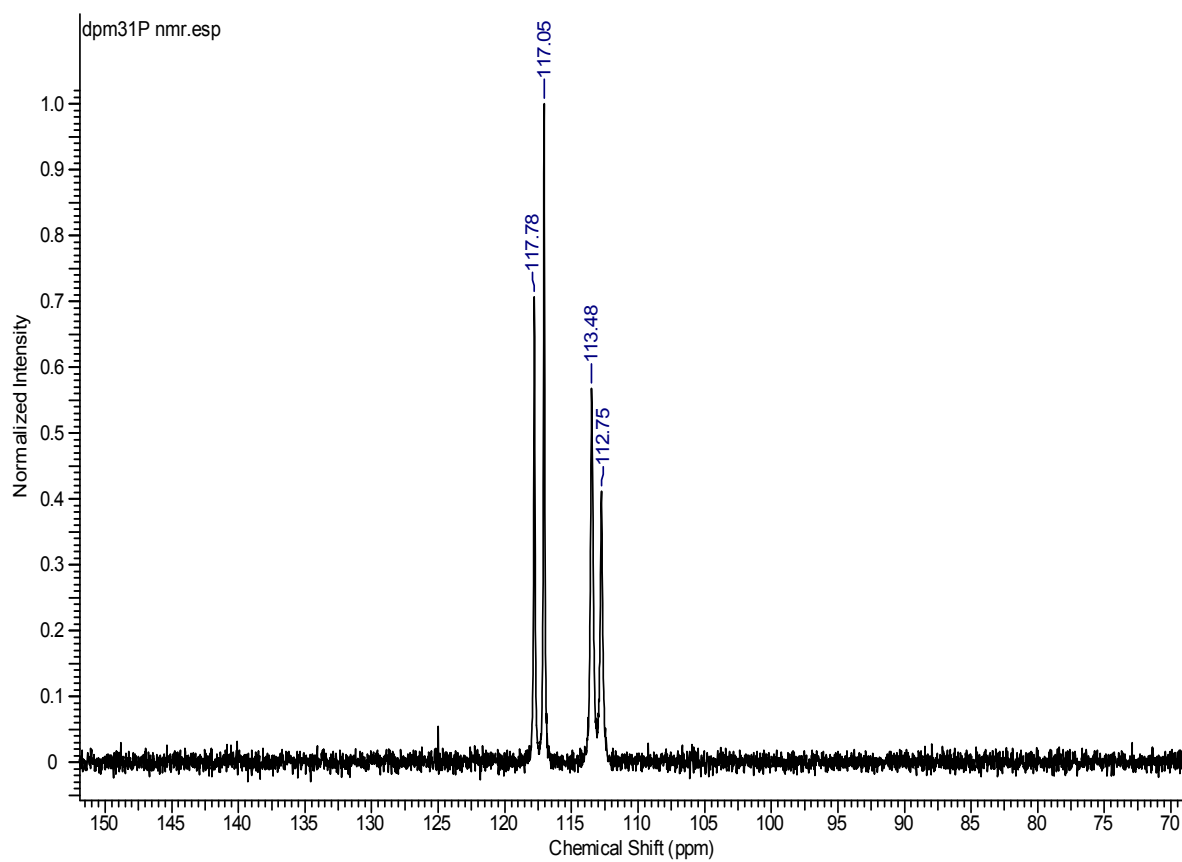
¹H NMR



¹¹B{¹H} NMR

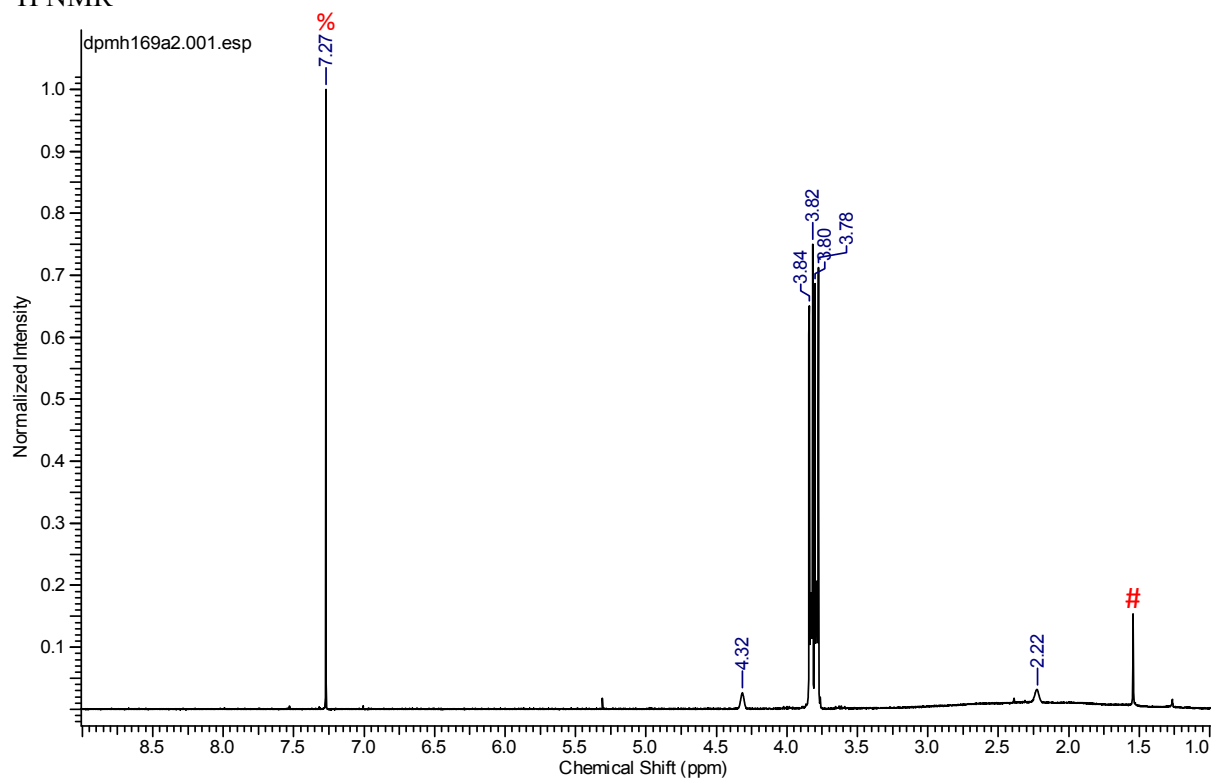


$^{31}\text{P}\{^1\text{H}\}$ NMR

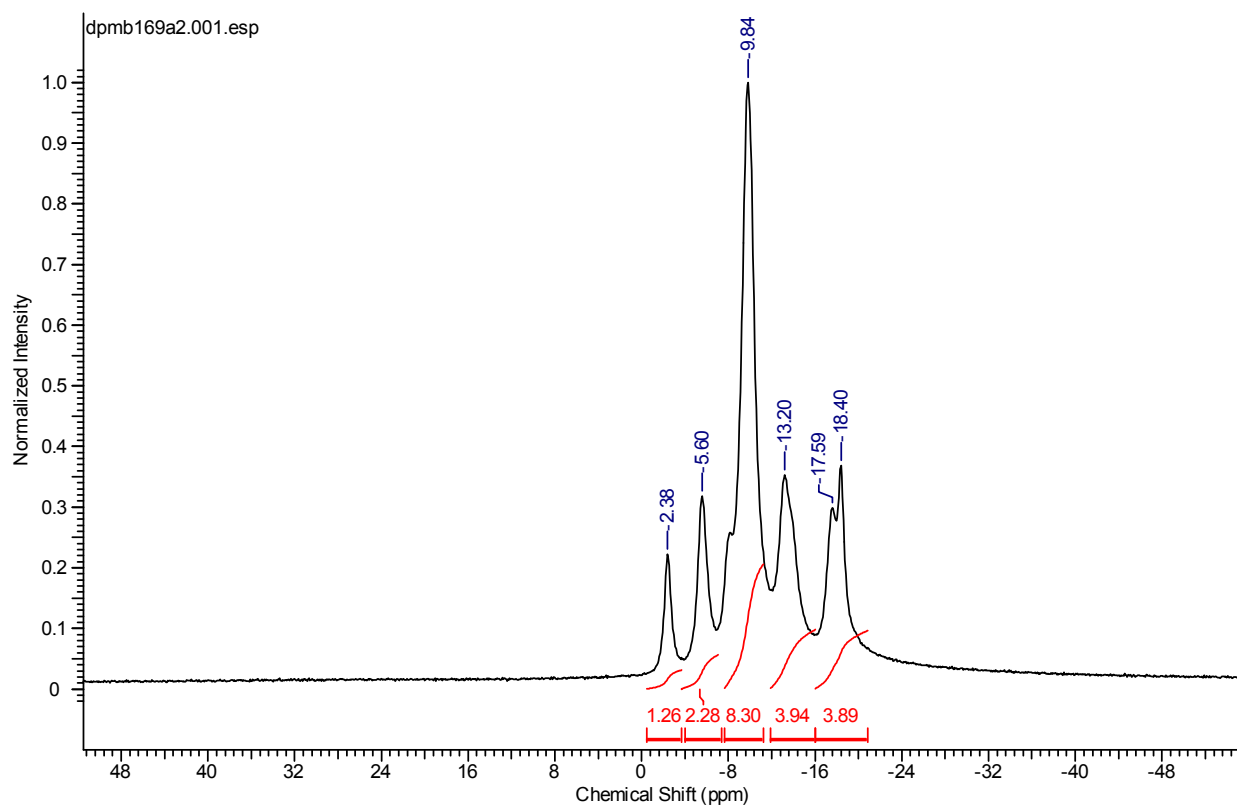


Compound **10**: [1-(1'-1',2'-*closo*-C₂B₁₀H₁₁)-2,2-{P(OMe)₃}₂-2,1,8-*closo*-NiC₂B₉H₁₀]

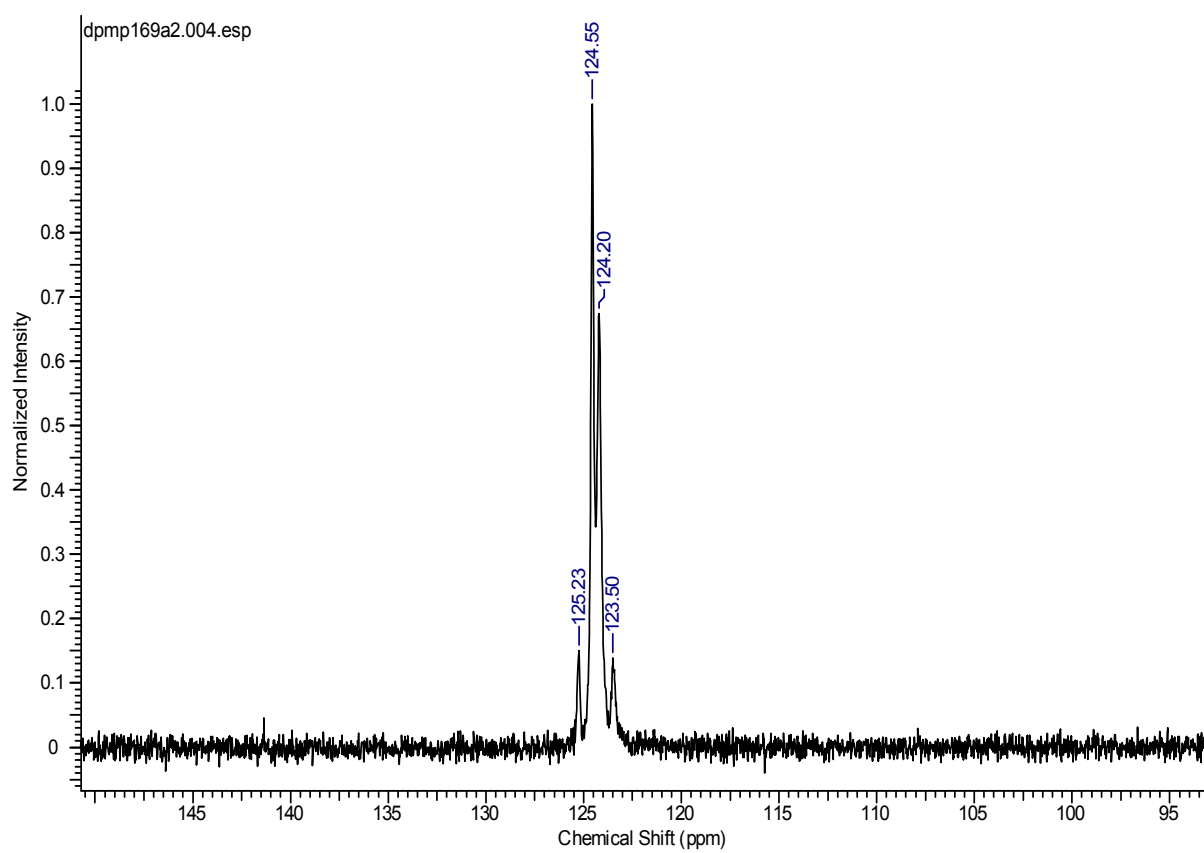
¹H NMR

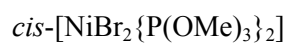


¹¹B{¹H} NMR

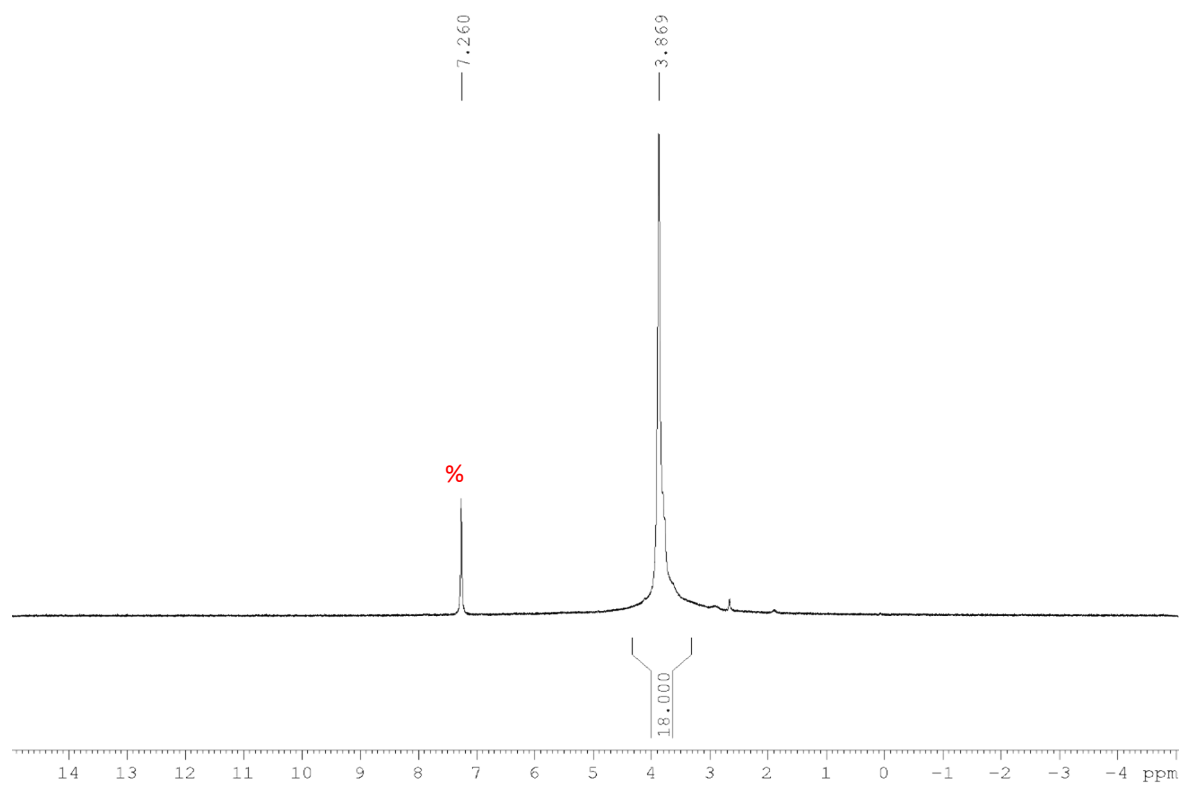


$^{31}\text{P}\{^1\text{H}\}$ NMR





¹H NMR



³¹P{¹H} NMR

