

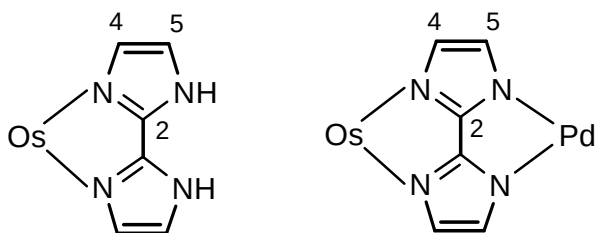
SUPPORTING INFORMATION

Title: Heterotrinnuclear Complexes of the Platinum Group Metals with 2,2'-Biimidazol as a Bridging Ligand

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NMR spectra of $[\text{Os}(\text{H}_2\text{biim})_2(\text{O}=\text{PPh}_3)_2](\text{NO}_3)_3$, **1** (H_2biim = 2,2'-biimidazole) and $[(\text{PdL})_2(\mu\text{-biim})_2\text{Os}(\text{O}=\text{PPh}_3)_2](\text{NO}_3)_3$ [**8**, L = cod, 1,5-cyclooctadiene; **9**, L = en, ethylen-1,2-diamine] were recorded at 300.135 MHz (^1H), 75.469 MHz ($^{13}\text{C}\{^1\text{H}\}$) or 121.495 MHz ($^{31}\text{P}\{^1\text{H}\}$) in CD_3OD . The relatively low solubility of these complexes in CD_3OD results in low intensities in the proton NMR spectra. Solubilities in DMSO or DMF are significantly higher. However, $[\text{D}^6]\text{DMSO}$ or $[\text{D}^7]\text{DMF}$ could not be used for the NMR spectra because triphenylphosphine oxide in **1**, **8** and **9** is easily substituted with these solvents. Spectra in CD_3OD allowed to determine chemical shifts of carbon or phosphorous in the coordinated 2,2'-biimidazole or triphenylphosphine oxide ligands. The NMR data are listed in Table 1 (atom numbering corresponds to Scheme 1). NMR spectra of **1**, **8** and **9**, are shown in Fig. 3 – 11 (signals of solvents are identified with *). NMR spectra of free 2,2'-biimidazole are given for comparison (Fig. 1, 2).



Scheme 1

Table 1. NMR data of metal-free 2,2'-biimidazole and triphenylphosphine oxide and in complexes **1**, **8** and **9**

Compound	$^{13}\text{C}\{^1\text{H}\}$ NMR		$^{31}\text{P}\{^1\text{H}\}$ NMR
	C-2, -2'	C-4, 4'	
H_2biim	139.4	128.3	-
$\text{Ph}_3\text{P}=\text{O}$	-	-	26.95
1	141.2	138.6	36.36
8	152.1	141.3	32.46
9	152.6	141.1	32.58

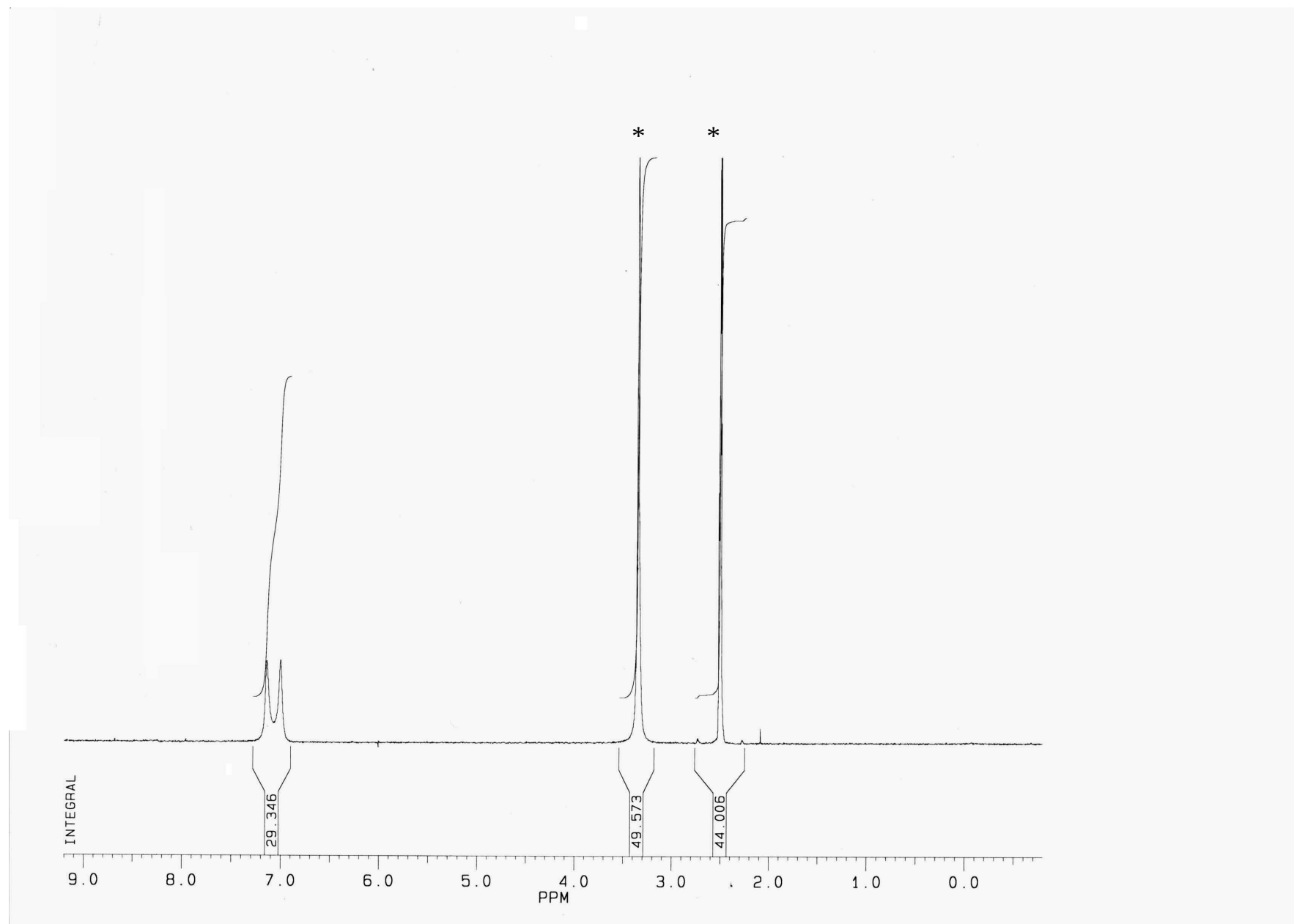


Figure 1. ^1H NMR spectrum of 2,2'-biimidazole in $[\text{D}^6]\text{DMSO}$.

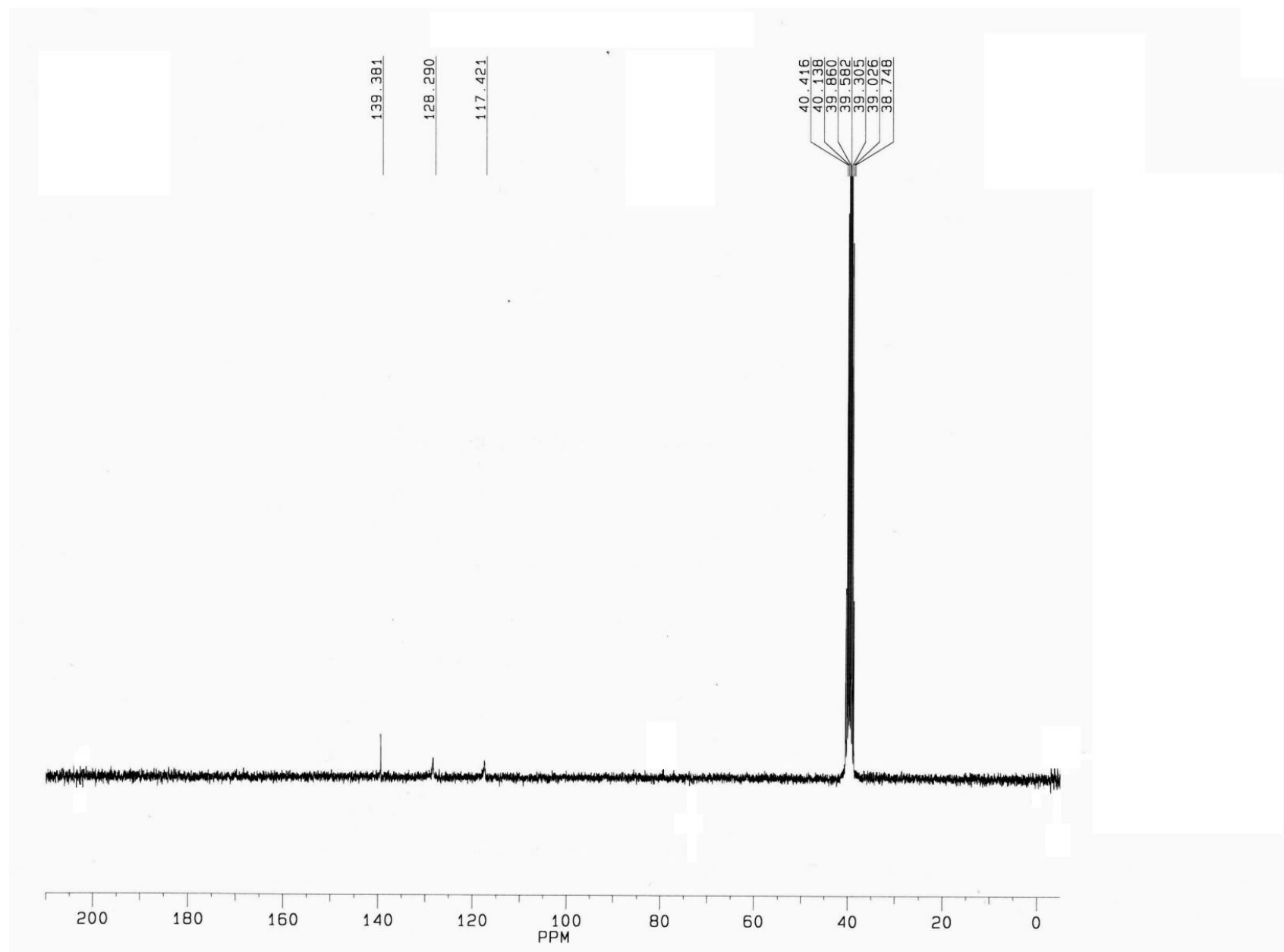


Figure 2. ¹³C{¹H} NMR spectrum of 2,2'-biimidazole in [D⁶]DMSO.

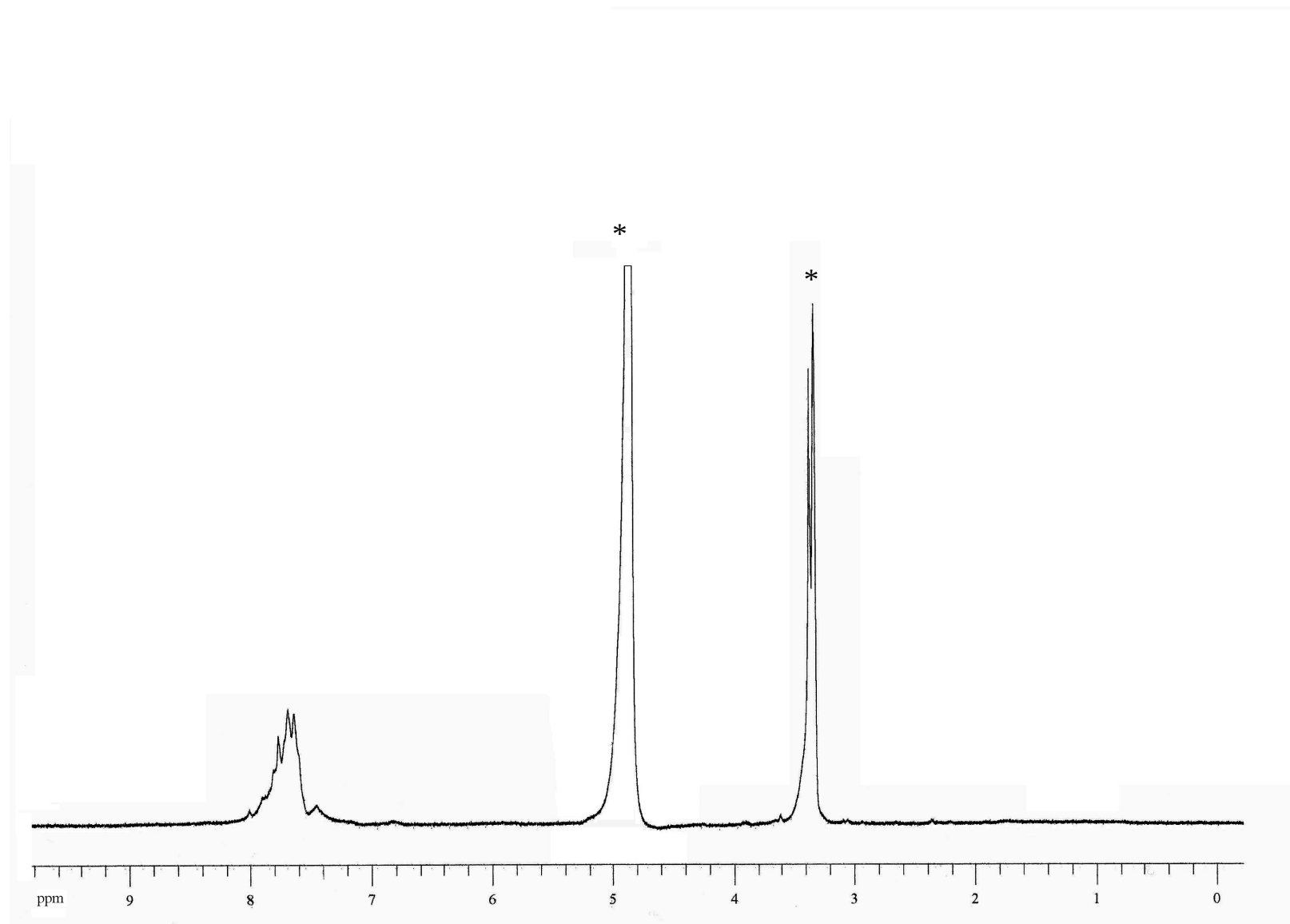


Figure 3. ^1H NMR spectrum of $[\text{Os}(\text{H}_2\text{biiim})_2(\text{O}=\text{PPh}_3)_2](\text{NO}_3)_3$ in CD_3OD .

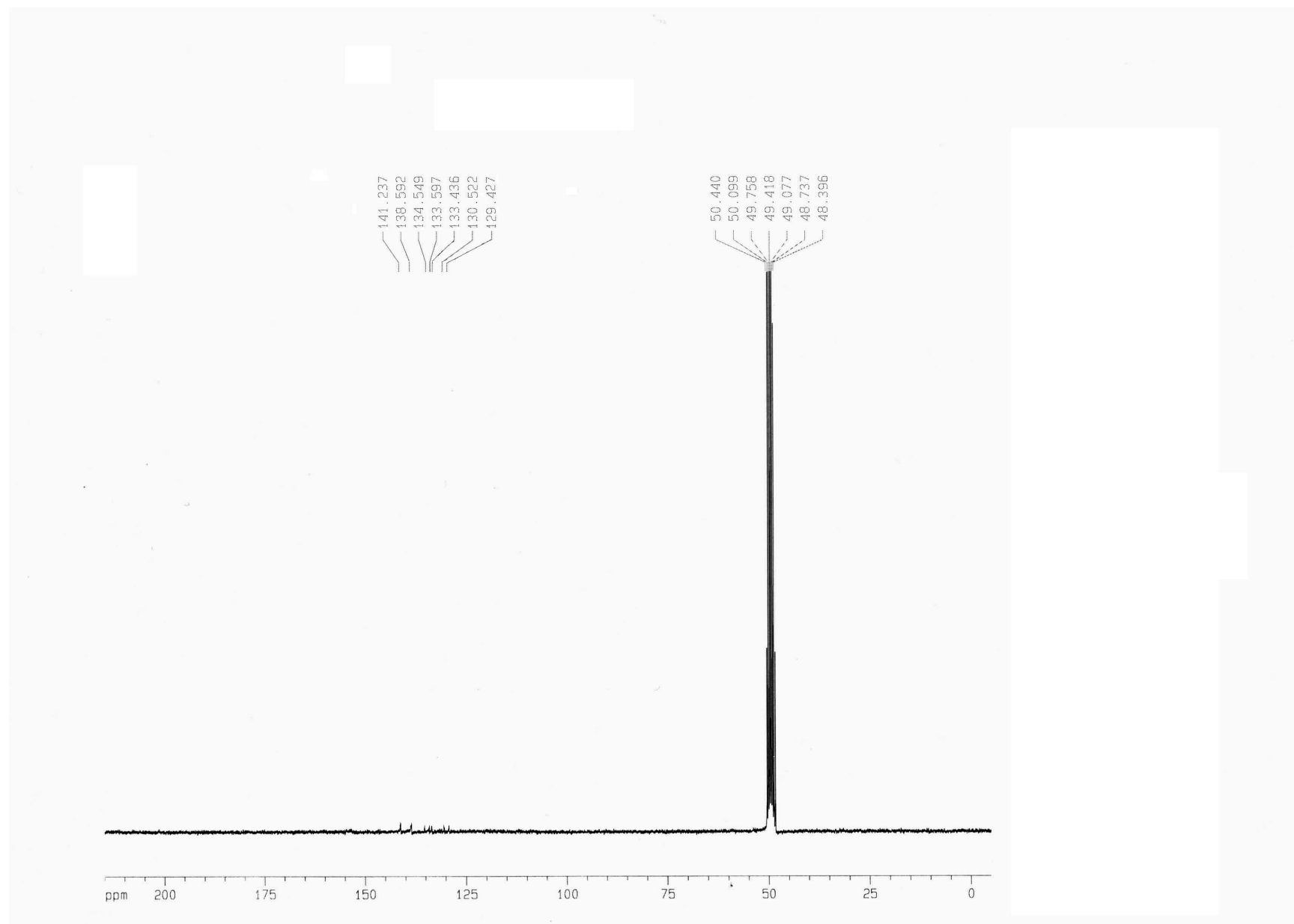


Figure 4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Os}(\text{H}_2\text{biim})_2(\text{O}=\text{PPh}_3)_2](\text{NO}_3)_3$ in CD_3OD .

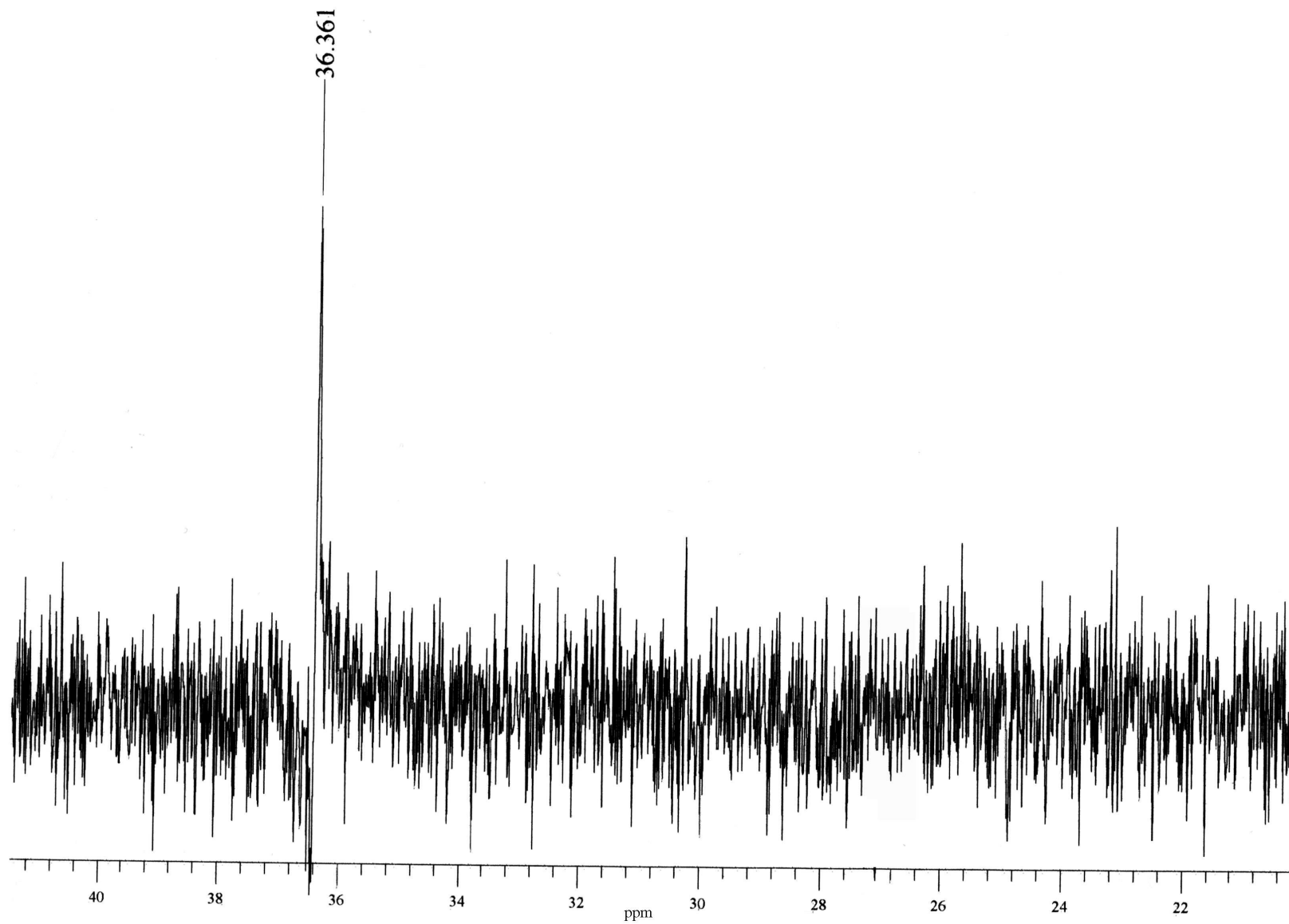


Figure 5. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\text{Os}(\text{H}_2\text{biim})_2(\text{O}=\text{PPh}_3)_2](\text{NO}_3)_3$ in CD_3OD .

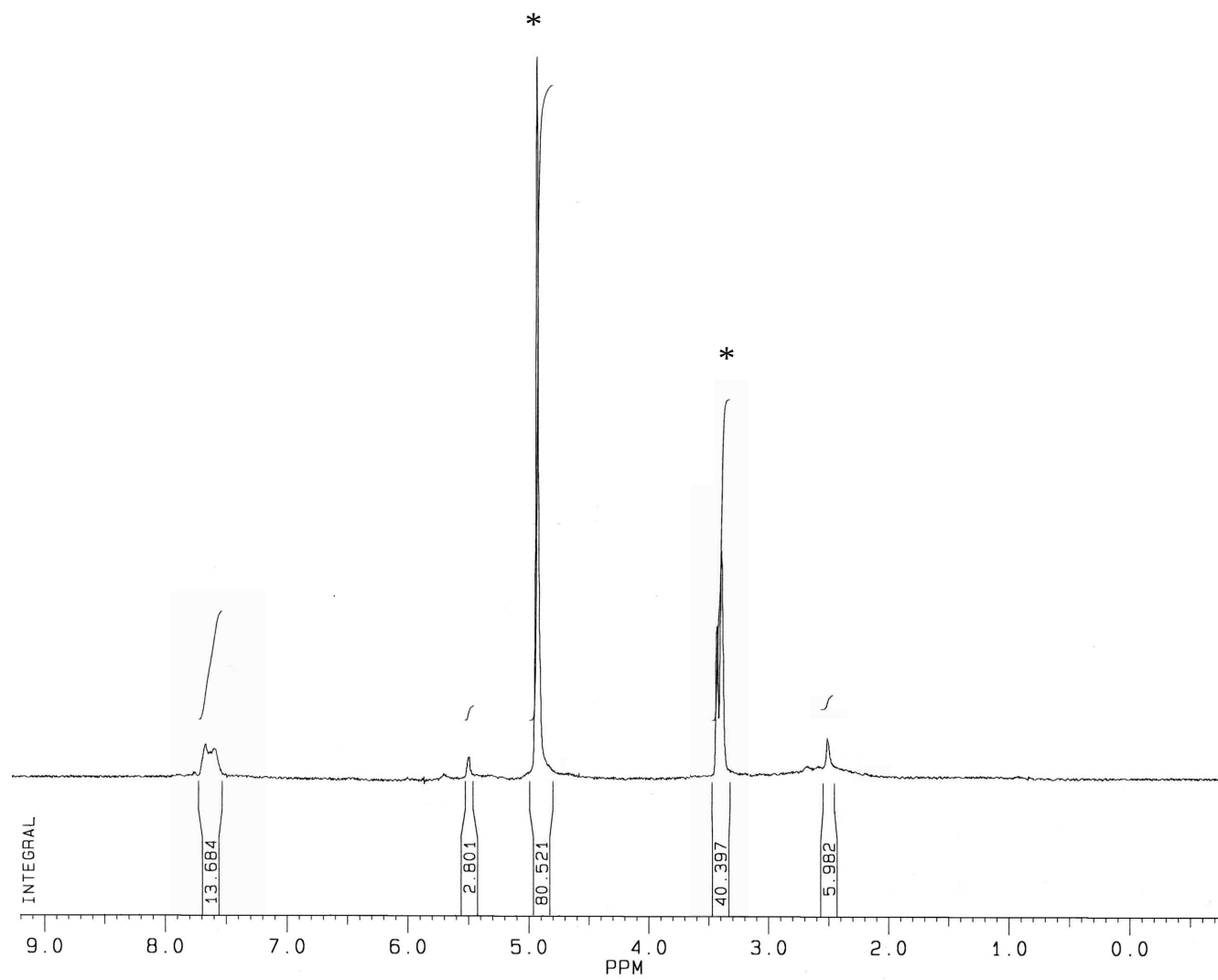


Figure 6. ^1H NMR spectrum of $[\{\text{Pd}(\text{cod})\}_2(\mu\text{-biim})_2\text{Os}(\text{O}=\text{PPh}_3)_2](\text{NO}_3)_3$ in CD_3OD .

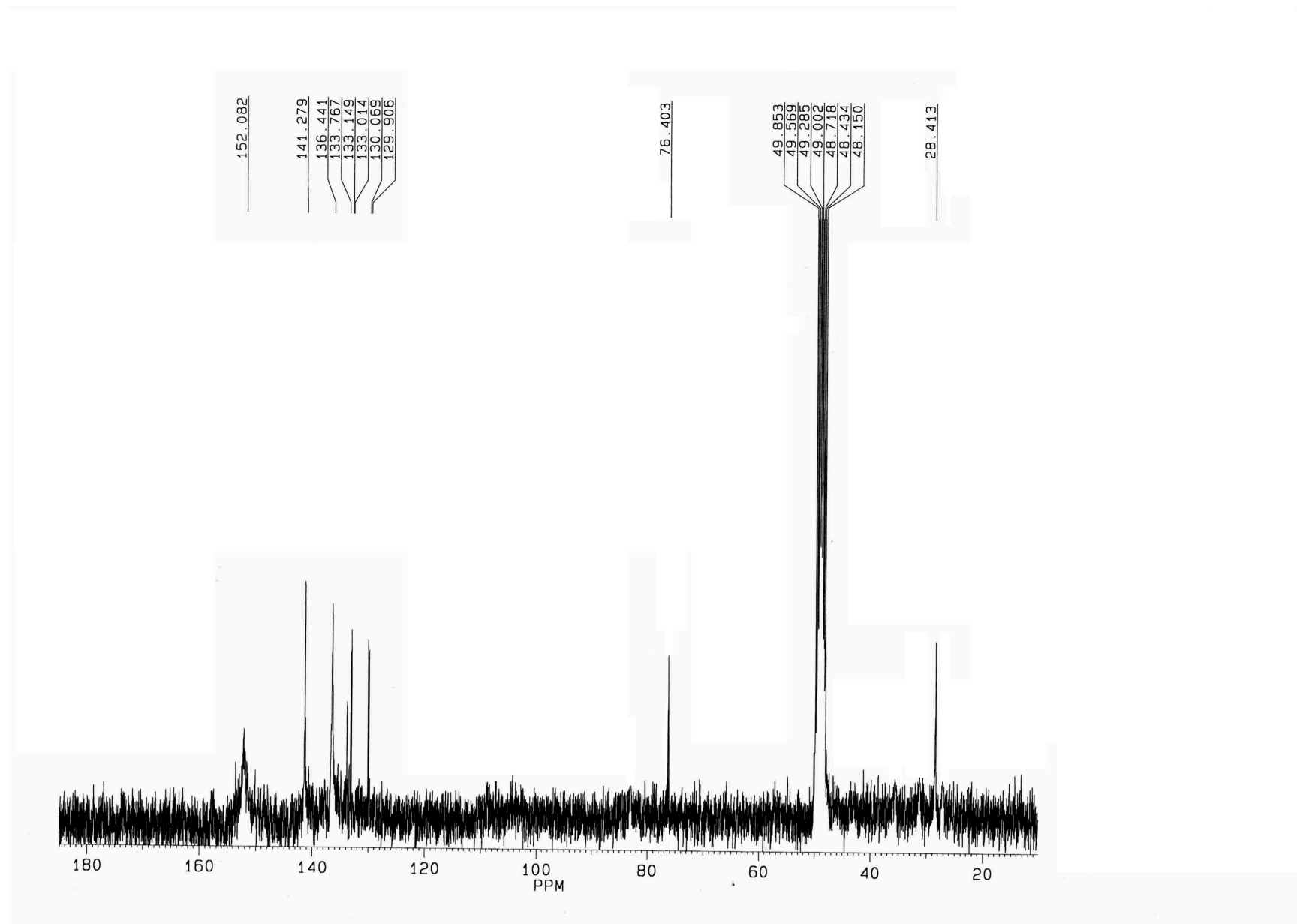


Figure 7. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\{\text{Pd}(\text{cod})\}_2(\mu\text{-biim})_2\text{Os}(\text{O}=\text{PPh}_3)_2](\text{NO}_3)_3$ in CD_3OD .

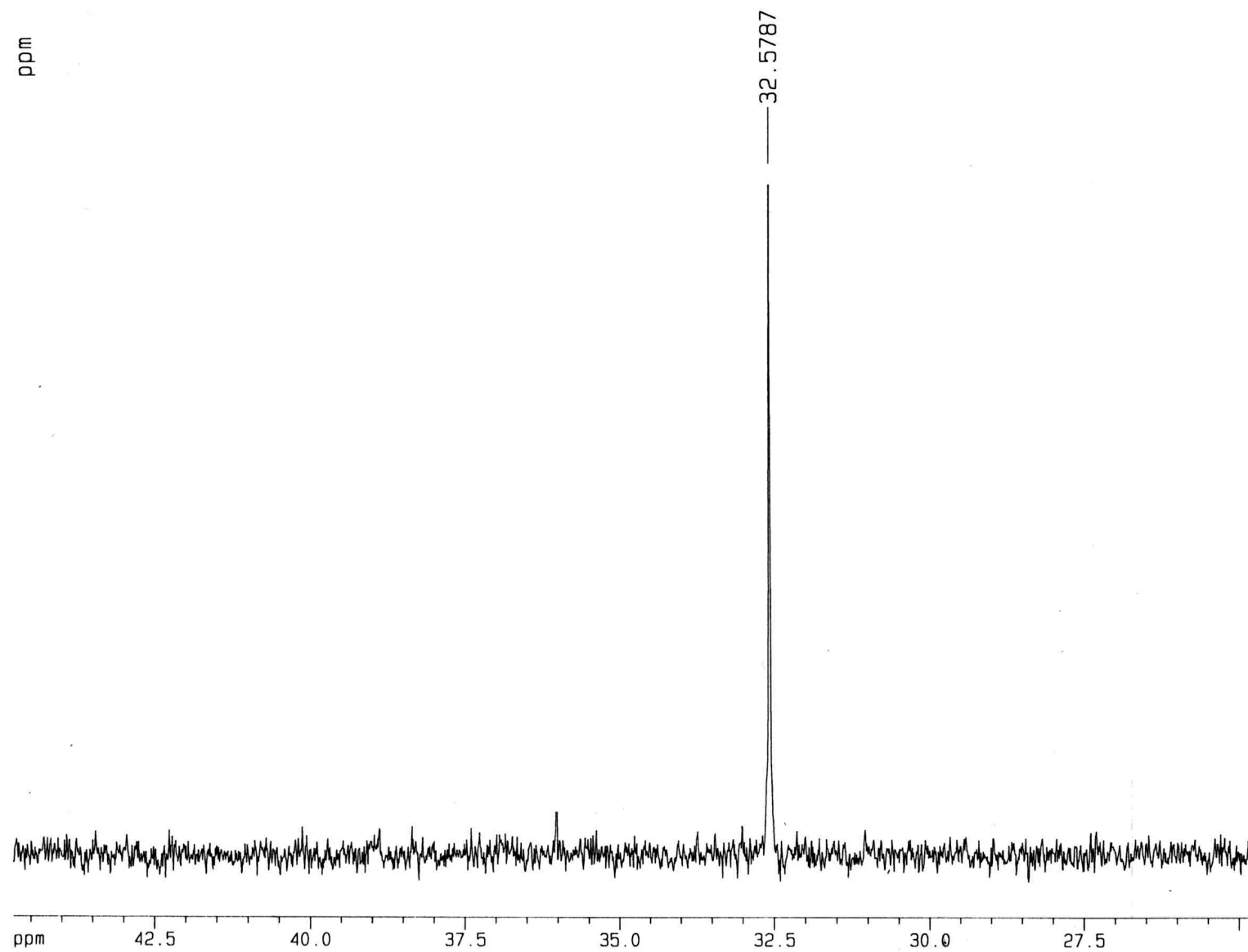


Figure 8. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\{\text{Pd}(\text{cod})\}_2(\mu\text{-biim})_2\text{Os}(\text{O}=\text{PPh}_3)_2](\text{NO}_3)_3$ in CD_3OD .

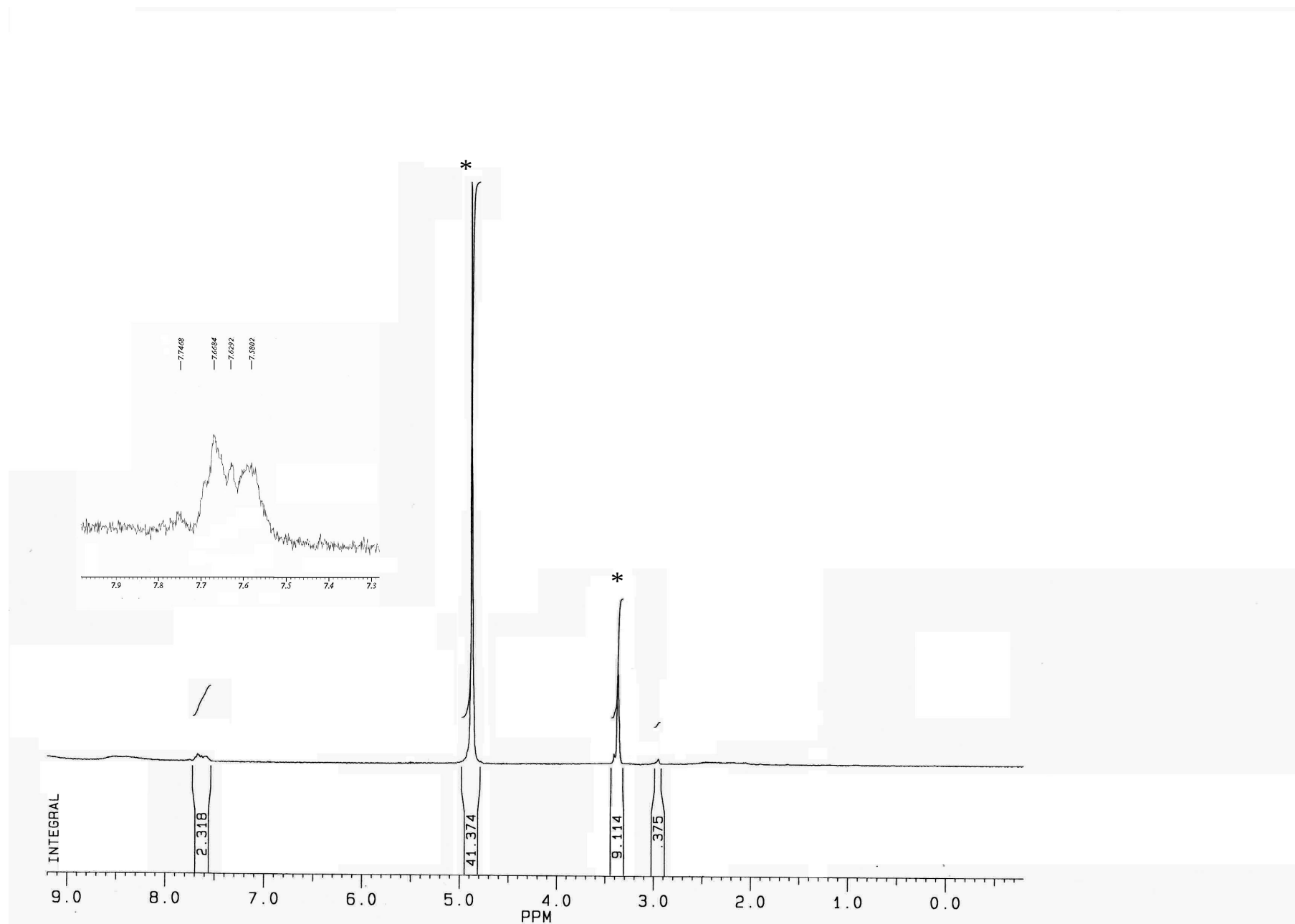


Figure 9. ^1H NMR spectrum of $[\{\text{Pd}(\text{en})\}_2(\mu\text{-biim})_2\text{Os}(\text{O}=\text{PPh}_3)_2](\text{NO}_3)_3$ in CD_3OD .

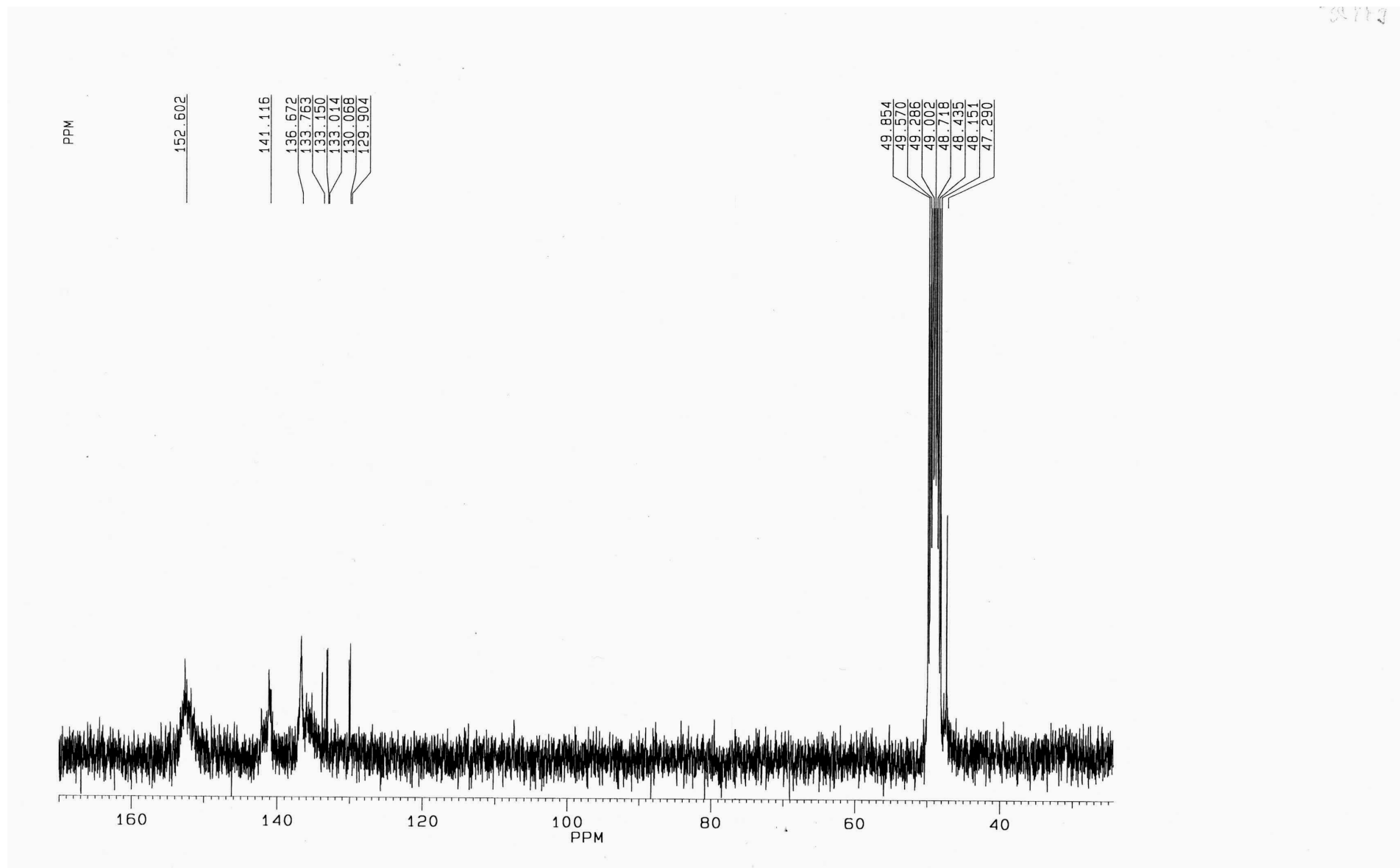


Figure 10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\{\text{Pd}(\text{en})\}_2(\mu\text{-biim})_2\text{Os}(\text{O}=\text{PPh}_3)_2](\text{NO}_3)_3$ in CD_3OD .

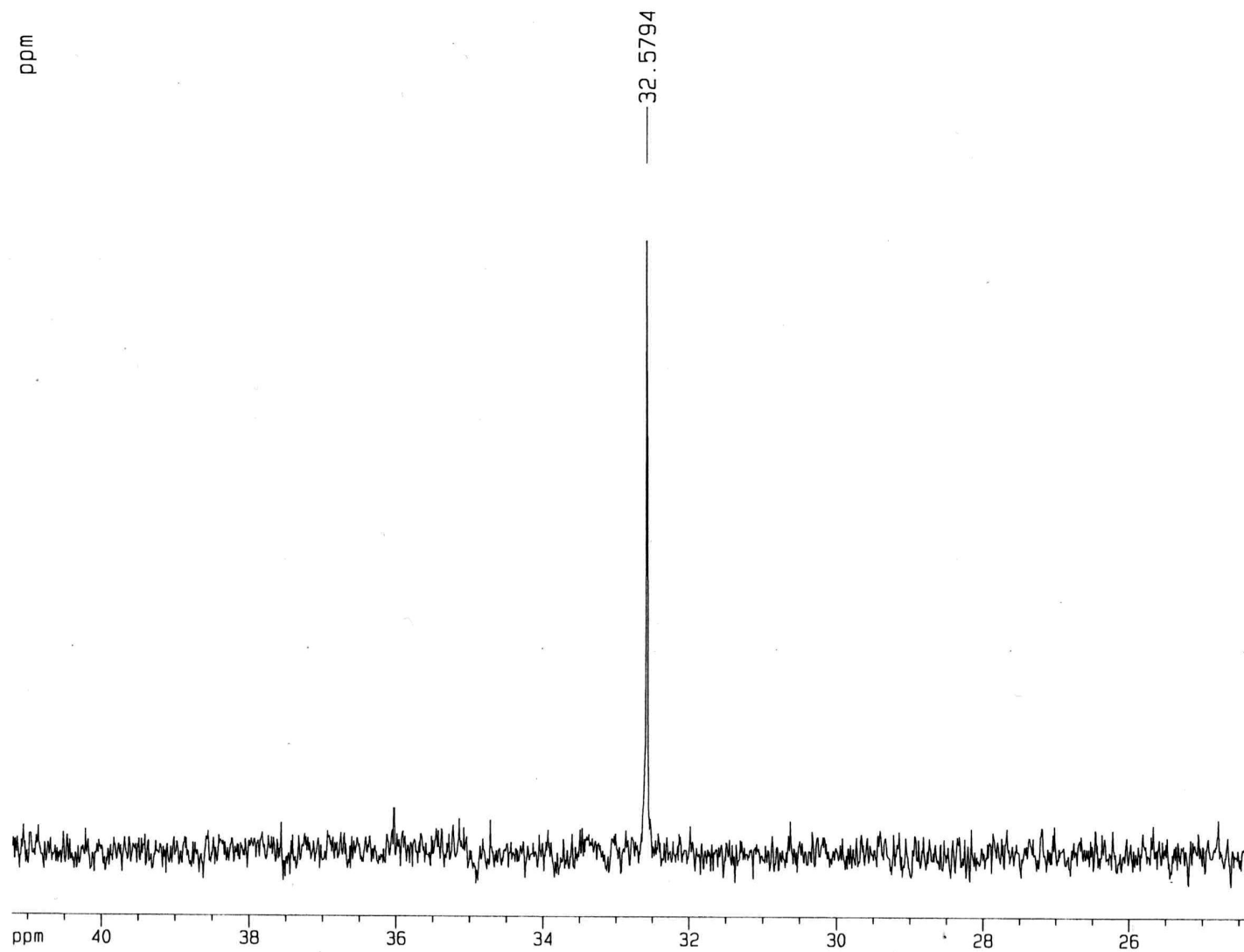


Figure 11. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\{\text{Pd}(\text{en})\}_2(\mu\text{-biim})_2\text{Os}(\text{O}=\text{PPh}_3)_2](\text{NO}_3)_3$ in CD_3OD .