

G. Albertin *et al.*, Preparation and Reactivity of Half-Sandwich Organic Azide Complexes of Osmium

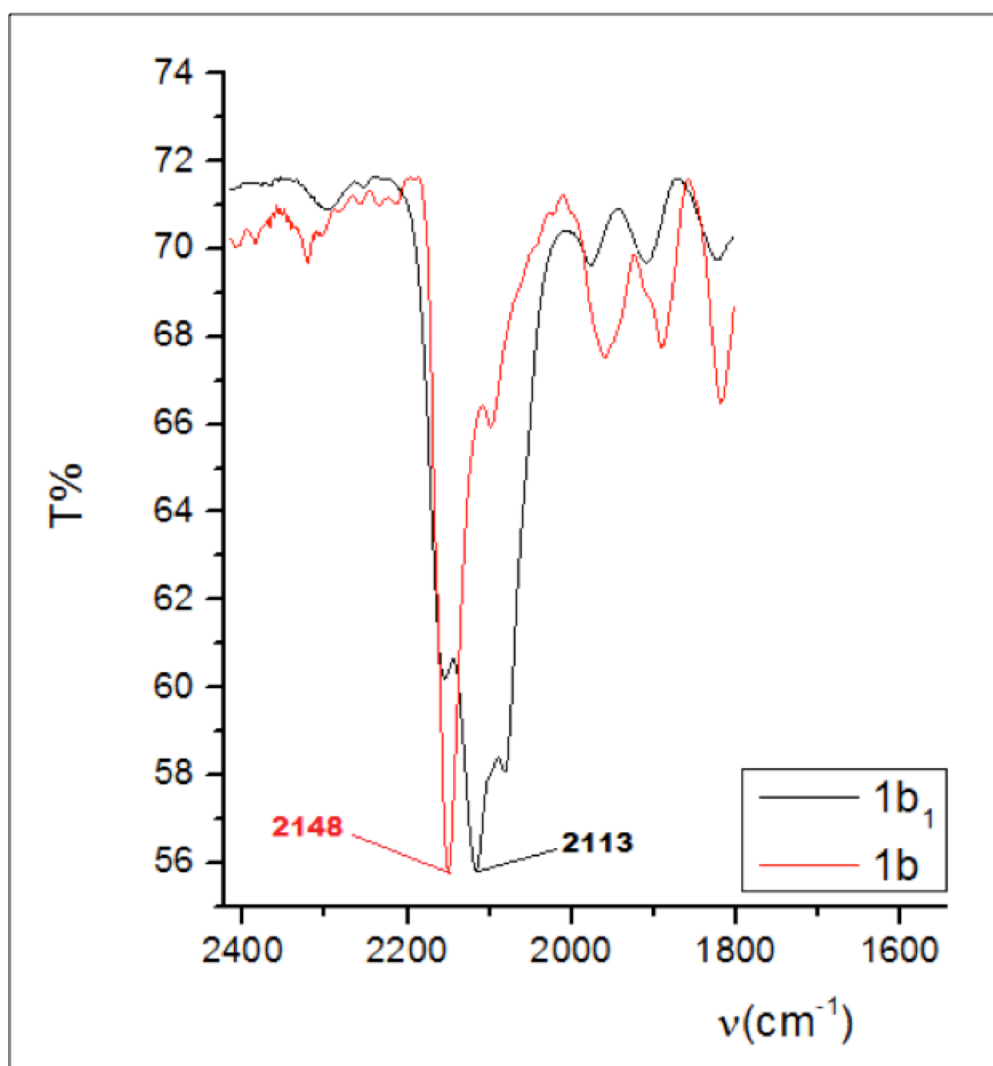


Figure S1. IR spectra of in KBr the labelled $[\text{Os}(\eta^5\text{-C}_5\text{H}_5)(\kappa^1\text{-}^{15}\text{N}_3\text{CH}_2\text{C}_6\text{H}_4\text{-4-CH}_3)(\text{PPh}_3)\text{-}\{\text{P}(\text{OMe})_3\}]\text{BPh}_4$ (**1b₁**) and unlabelled compound $[\text{Os}(\eta^5\text{-C}_5\text{H}_5)(\kappa^1\text{-N}_3\text{CH}_2\text{C}_6\text{H}_4\text{-4-CH}_3)(\text{PPh}_3)\text{-}\{\text{P}(\text{OMe})_3\}]\text{BPh}_4$ (**1b**).

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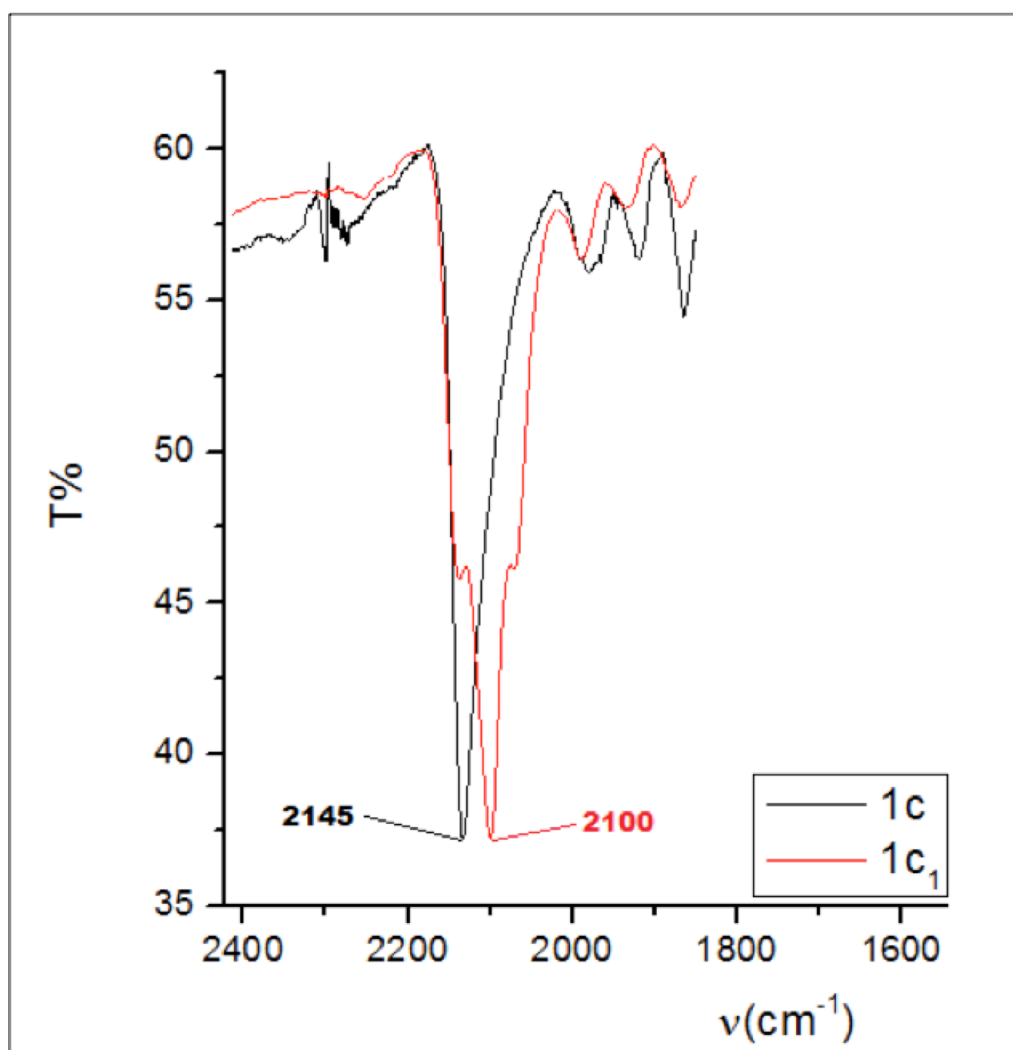


Figure S2. IR spectra of in KBr the labelled $[\text{Os}(\eta^5\text{-C}_5\text{H}_5)\{\kappa^1\text{-}^{15}\text{N}_3\text{C}(\text{H})(\text{CH}_3)\text{C}_6\text{H}_5\}(\text{PPh}_3)\{\text{P}(\text{OMe})_3\}]\text{BPh}_4$ (**1c**₁) and unlabelled compound $[\text{Os}(\eta^5\text{-C}_5\text{H}_5)\{\kappa^1\text{-N}_3\text{C}(\text{H})(\text{CH}_3)\text{C}_6\text{H}_5\}(\text{PPh}_3)\{\text{P}(\text{OMe})_3\}]\text{BPh}_4$ (**1c**).

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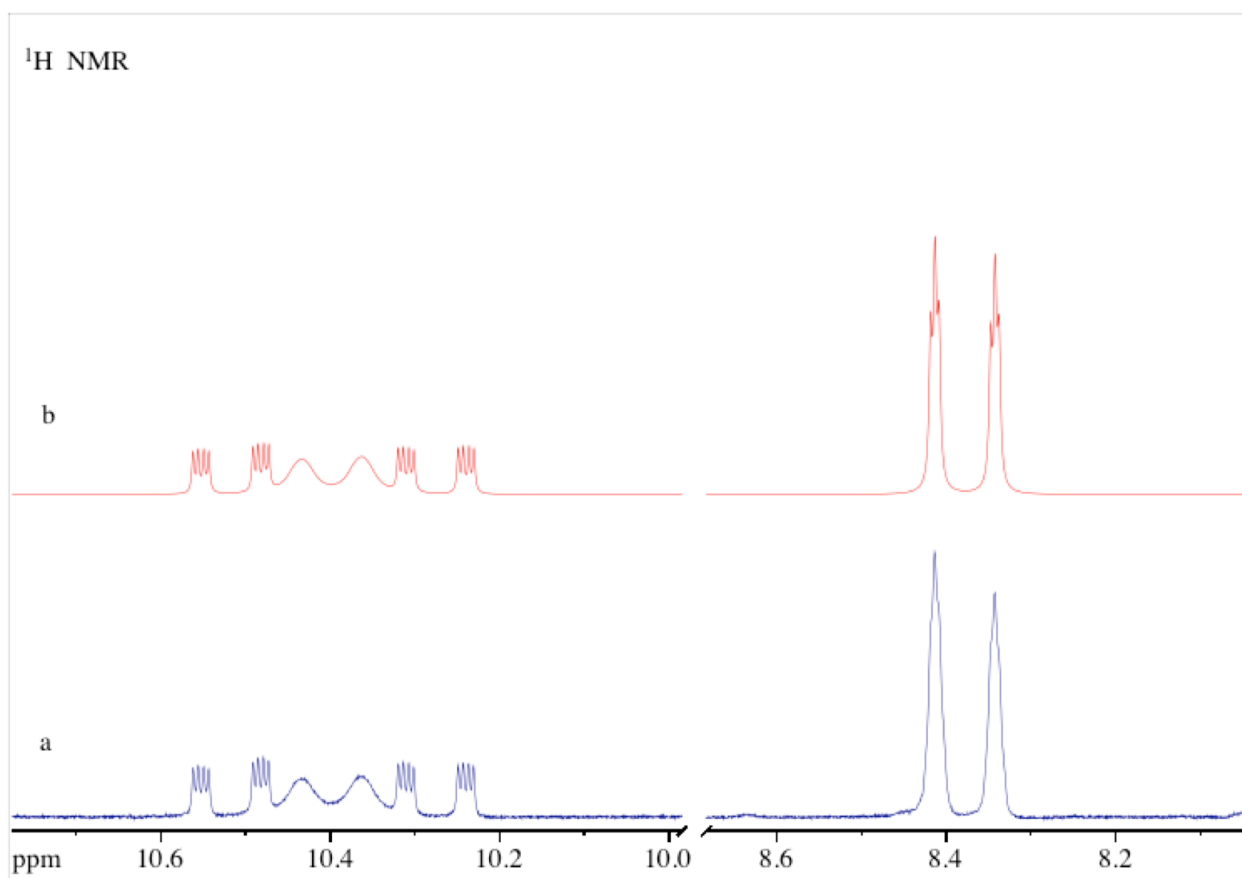


Figure S3. ^1H NMR spectra of complex $[\text{Os}(\eta^5\text{-C}_5\text{H}_5)\{\kappa^1\text{-}^{15}\text{NH}=\text{C}(\text{CH}_3)\text{C}_6\text{H}_4\text{-4-CH}_3\}(\text{PPh}_3)\text{-}\{\text{P}(\text{OMe})_3\}]\text{BPh}_4$ (**3b₁**) in CD_2Cl_2 at 295 K. Lower, experimental; upper, simulated (see parameters in Experimental section).

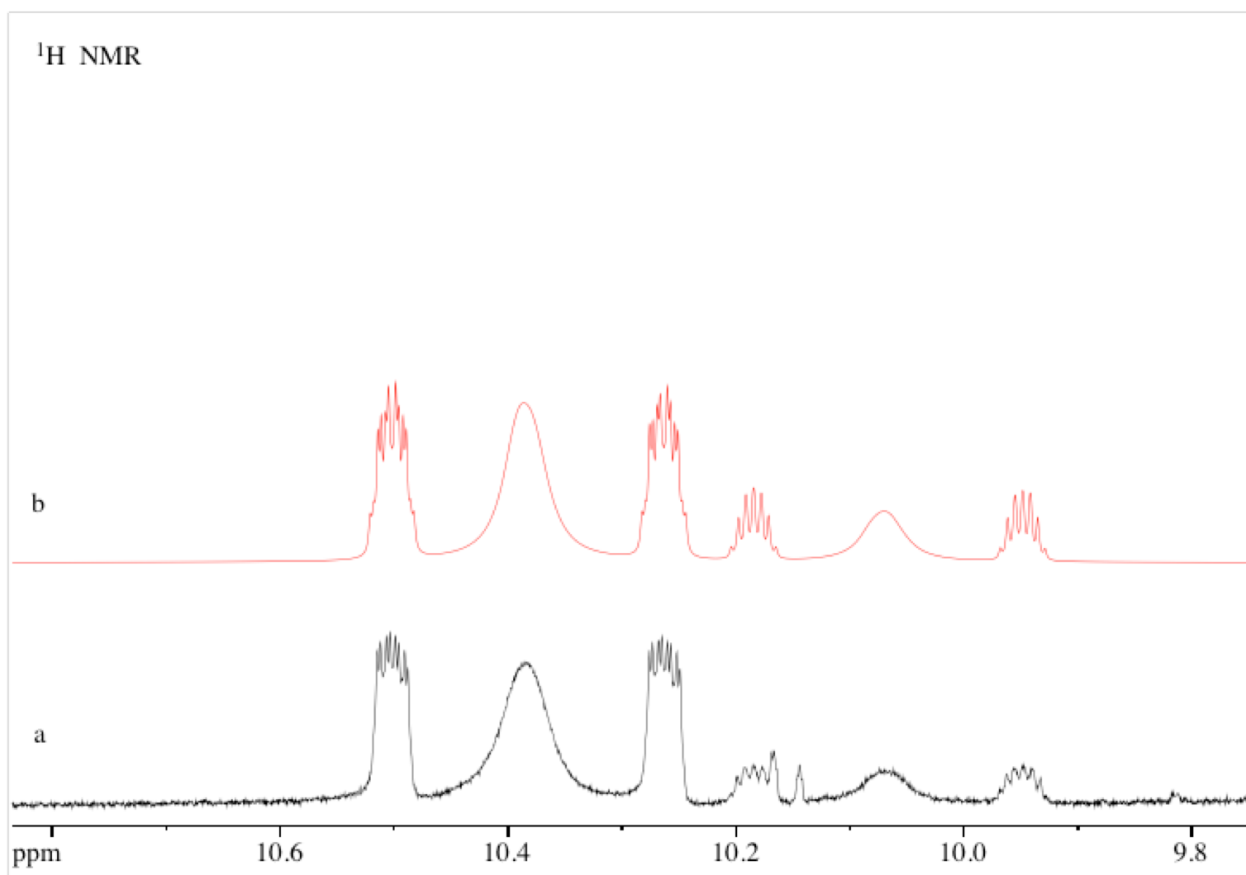
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Figure S4. ^1H NMR spectra of complex $[\text{Os}(\eta^5\text{-C}_5\text{H}_5)\{\kappa^1\text{-}^{15}\text{NH}=\text{C}(\text{CH}_3)\text{C}_6\text{H}_5\}(\text{PPh}_3)\text{-}\{\text{P}(\text{OEt})_3\}]\text{BPh}_4$ (**4c1**) in CD_2Cl_2 at 295 K. Lower, experimental; upper, simulated (see parameters in Experimental section).

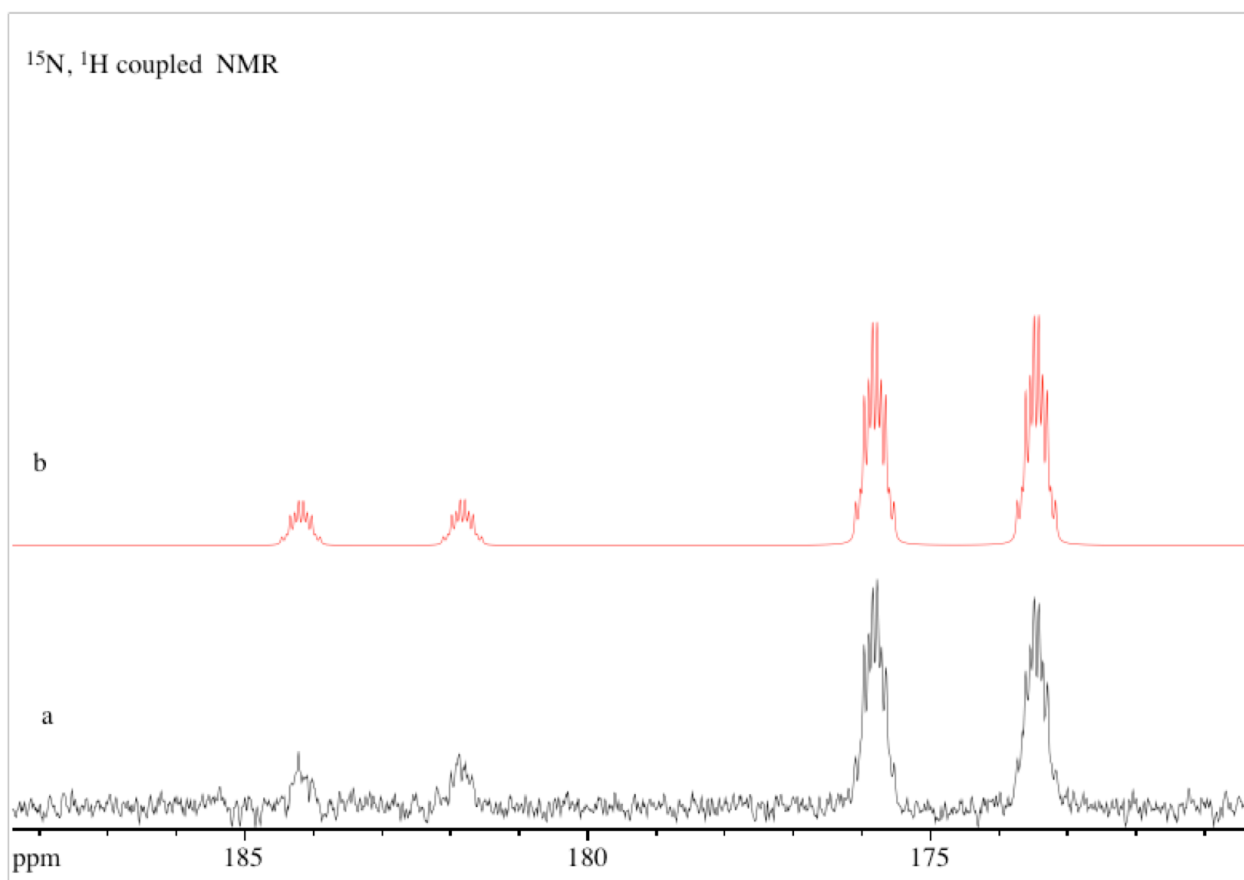
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Figure S5. Proton-coupled ¹⁵N NMR spectra of complex [Os(η⁵-C₅H₅){κ¹-¹⁵NH=C(CH₃)C₆H₅}(PPh₃){P(OEt)₃}]BPh₄ (**4c**₁) in CD₂Cl₂. Lower, experimental; upper, simulated (see parameters in Experimental section).