Di- and Tetrametallic Hafnocene Oxamidides Prepared from CO-Induced N₂ Bond Cleavage and Thermal Rearrangement to Hafnocene Cyanide Derivatives.

Scott P. Semproni, Grant W. Margulieux and Paul J. Chirik*

Department of Chemistry, Princeton University, Princeton, New Jersey, 08544

pchirik@princeton.edu

Supporting Information

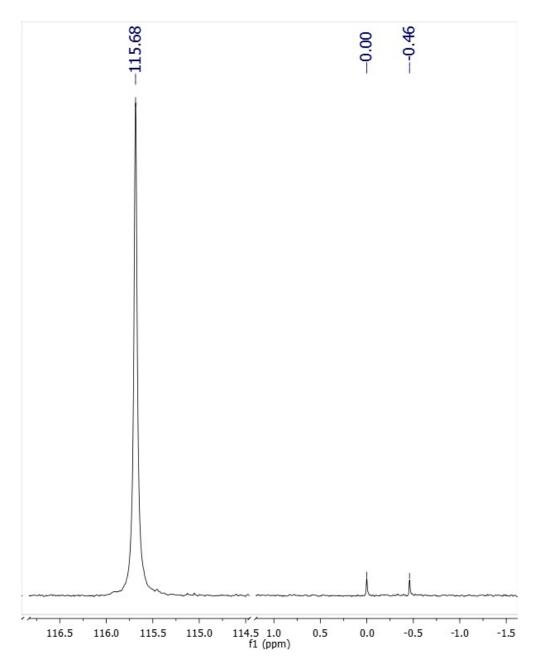


Figure S1. 13 C NMR spectrum of CH₃ 13 CN in benzene- d_6 at 23 $^{\circ}$ C.

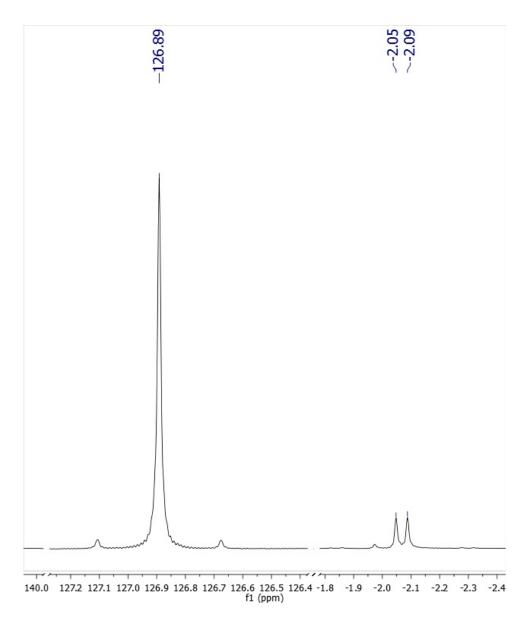


Figure S2. ¹³C NMR spectrum of Me₃Si¹³CN in benzene- d_6 at 23 °C.

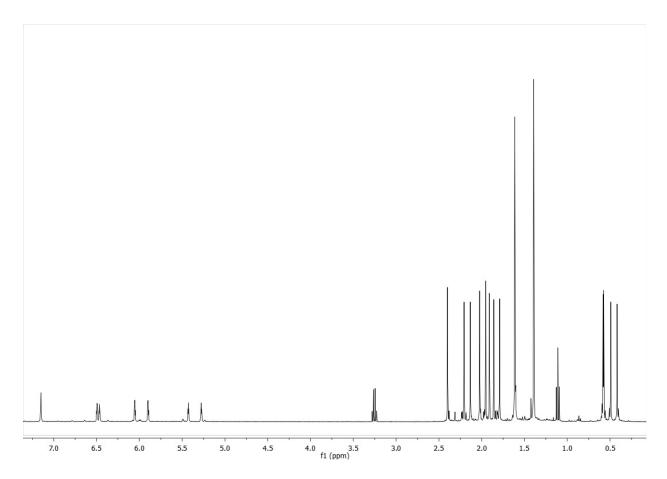
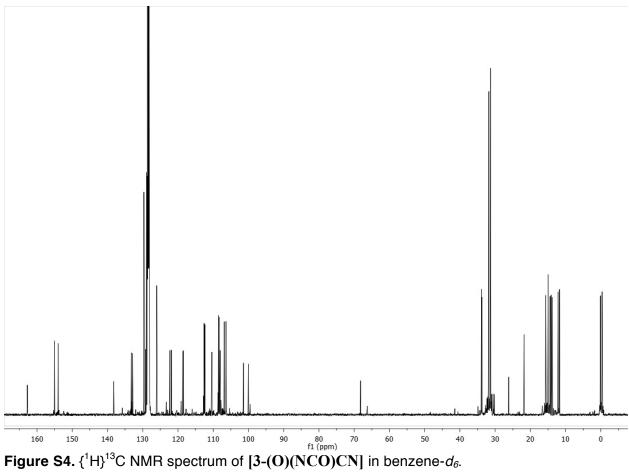


Figure S3. ¹H NMR spectrum of [3-(O)(NCO)CN] in benzene- d_6 .



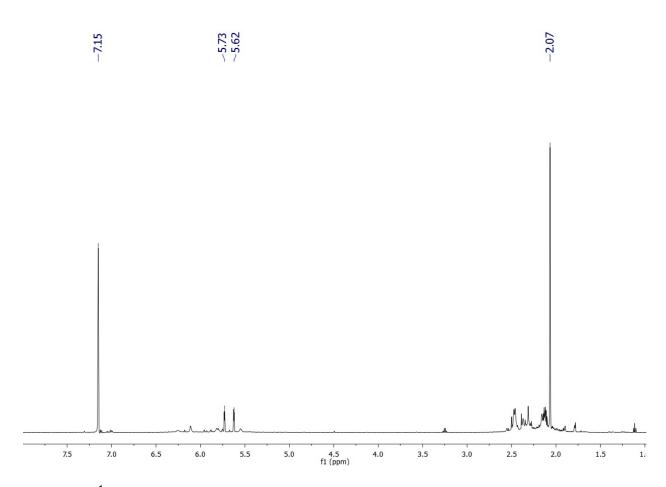


Figure S5. ¹H NMR spectrum of $[1-(NCO)]_2$ in benzene- d_6 .

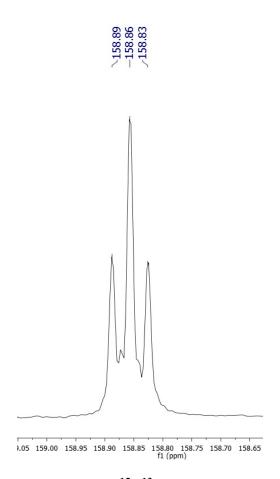


Figure S6. $\{^1H\}^{13}C$ NMR spectrum of $[1-(^{15}N^{13}CO)]_2$ in benzene- d_6 .

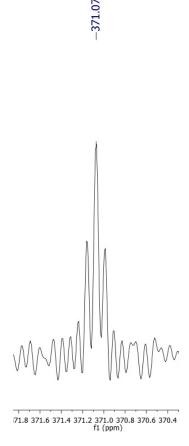
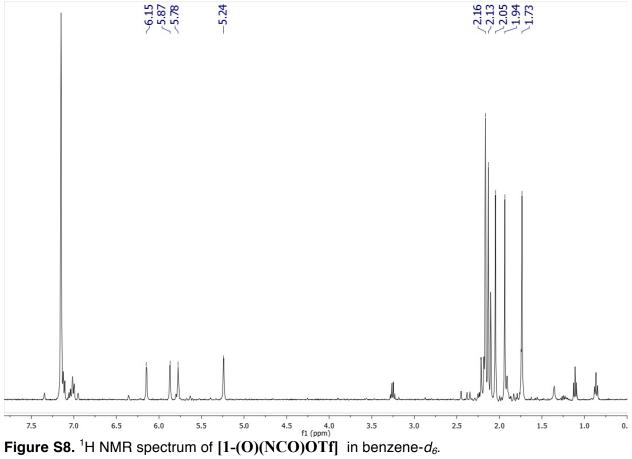


Figure S7. $\{^1H\}^{15}N$ NMR spectrum of $[1-(^{15}N^{13}CO)]_2$ in benzene- d_6 .



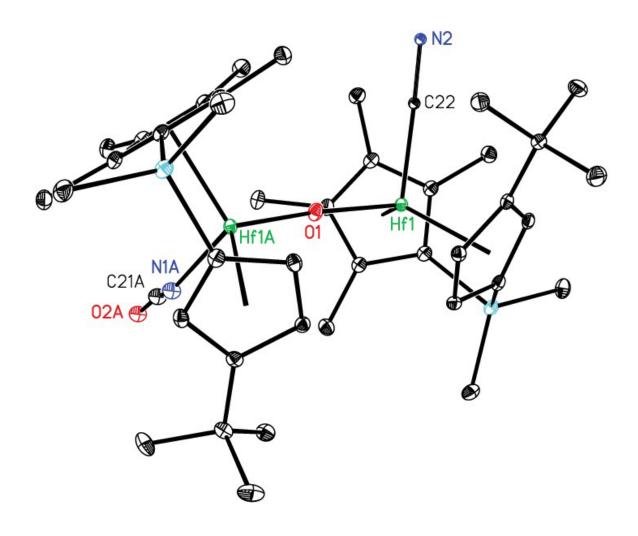


Figure S9. Representation of the solid state structure of (*R*, *R*)-[3-(O)(NCO)CN] at 30% probability ellipsoids. Solvent, hydrogen atoms and disordered cyanide/isocyanate groups omitted for clarity.