Electronic Supplementary Material (ESI) for Dalton Transactions.

Reactivity of Parent Amido Complexes of Iridium with Olefins: C–NH_2 Bond Formation *versus* C-H Activation

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Supporting Material

Figure S1. *In situ* ^{1}H NMR spectrum of **3** in C_6D_6 at 25 ^{o}C.

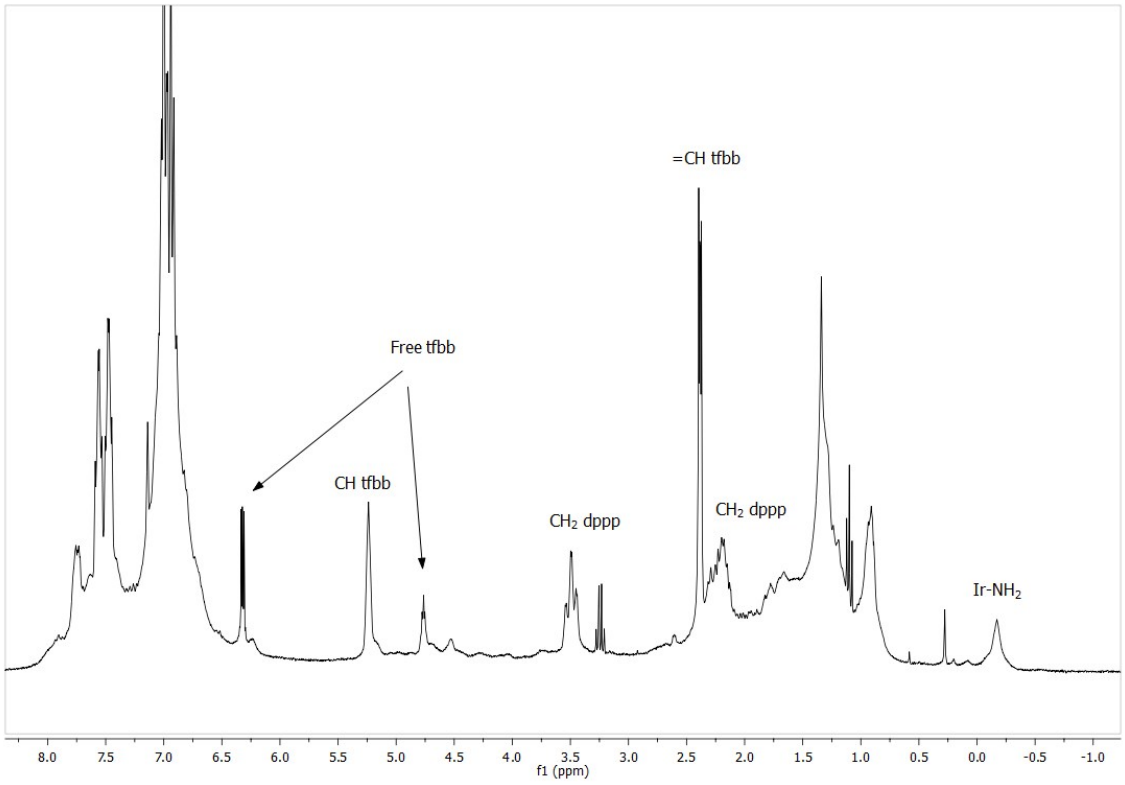


Figure S2. *In situ* $^{31}P\{^{1}H\}$ NMR spectrum of **3** in C_6D_6 at 25 ^{o}C.

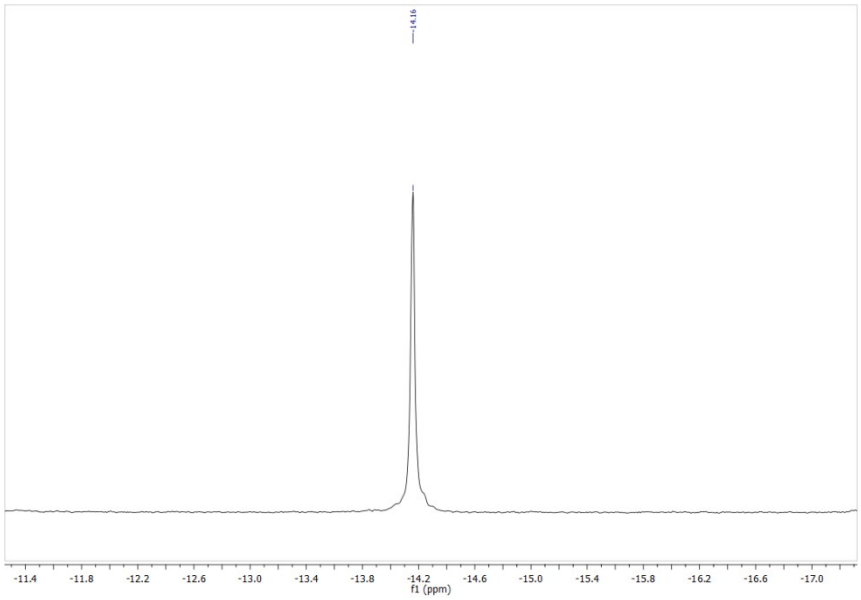


Figure S3. ^{1}H NMR spectrum of **4** in $CDCl_3$ at 25 ^{o}C.

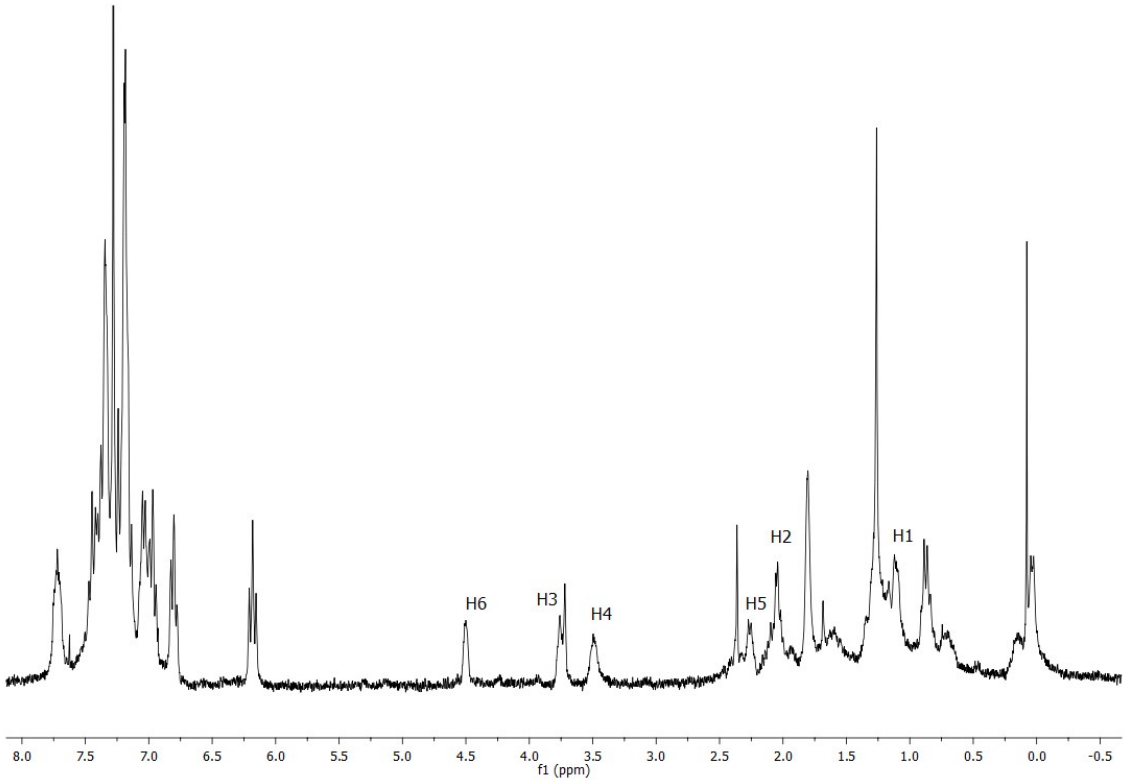


Figure S4. $^{31}P\{^{1}H\}$ NMR spectrum of **4** in $CDCl_3$ at 25 ^{o}C.

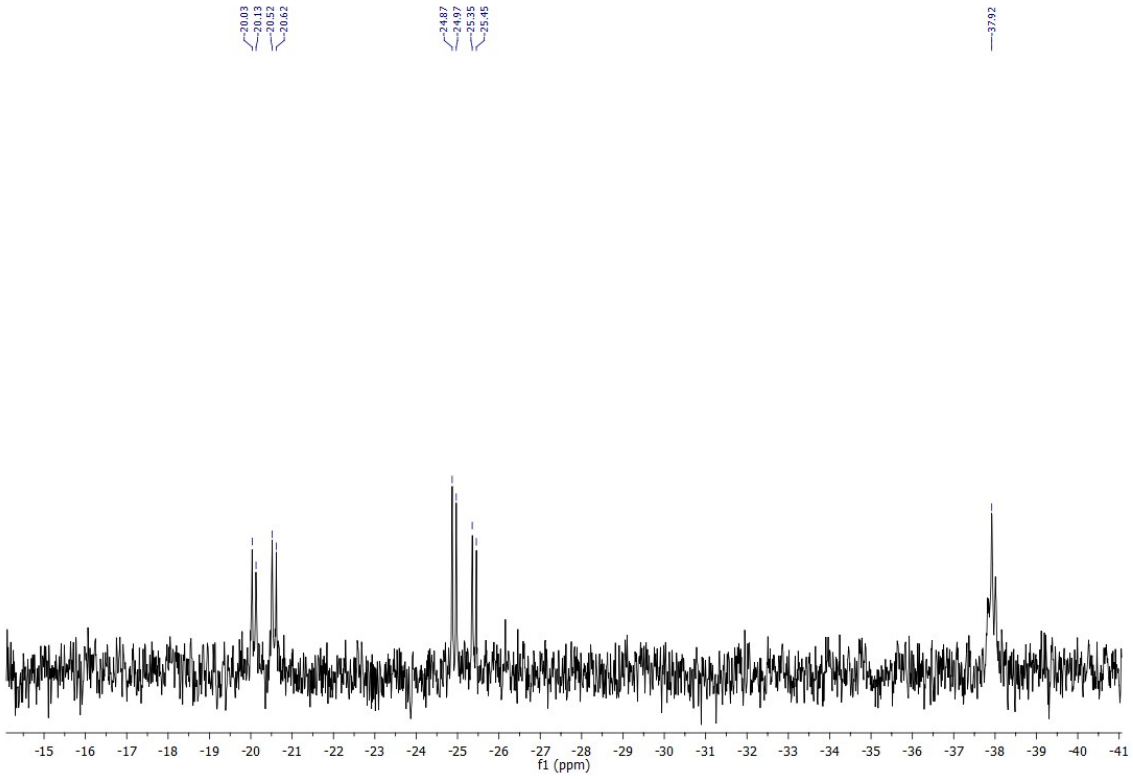


Figure S5. ^{1}H-^{1}H COSY NMR spectrum of **4** in $CDCl_3$at 25 ^{o}C.

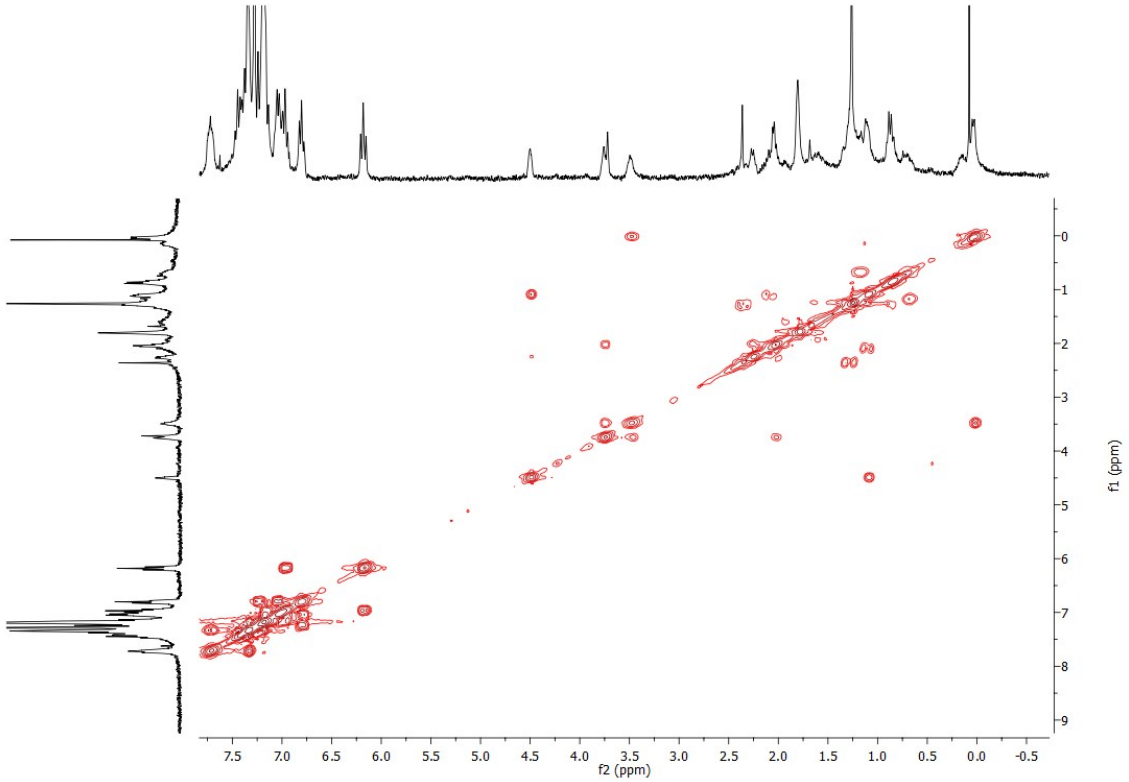


Figure S6. ^{1}H NMR spectrum of **5** in C_6D_6 at 25 ^{o}C (left) and detail of the hydrido area (right).

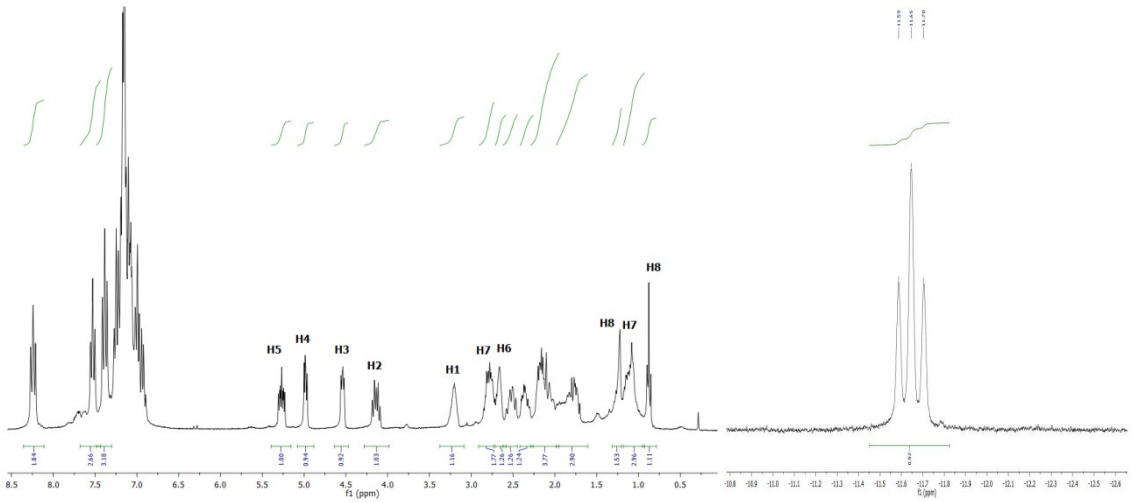


Figure S7. Selected region of the ^{1}H-^{1}H COSY NMR spectrum of **5** in C_6D_6 at 25 °C.

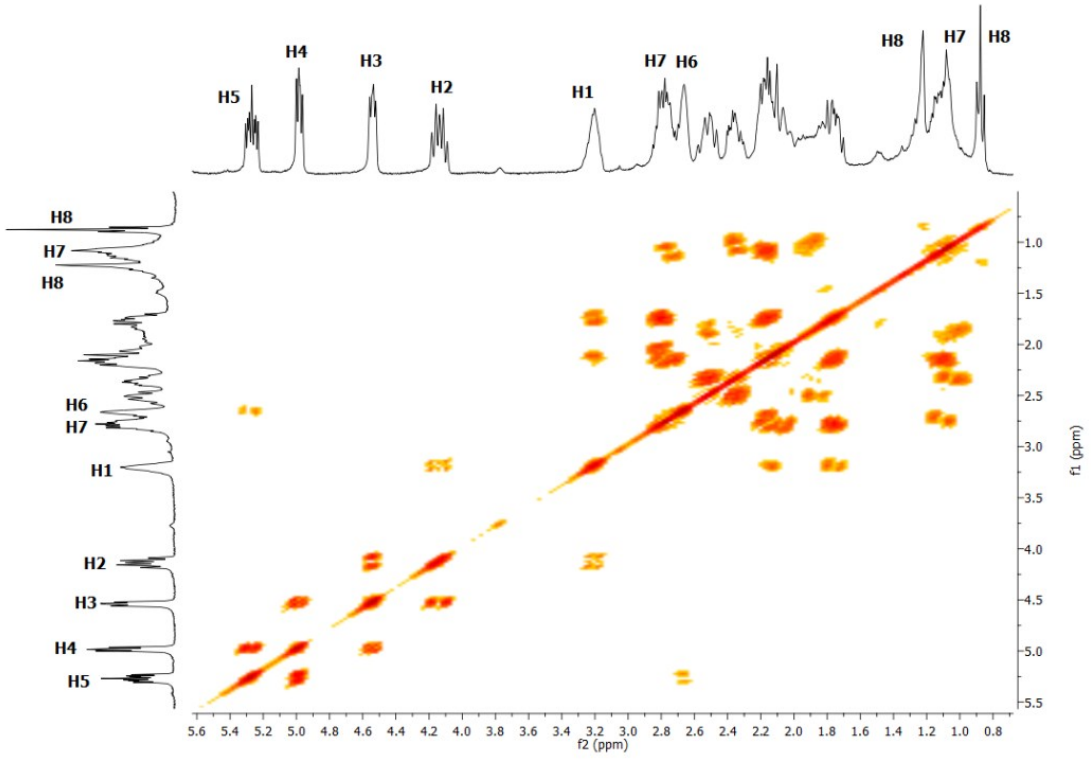


Figure S8. Selected region of the $^{13}C\{^{1}H\}$-APT NMR spectrum of **5** in C_6D_6 at 25 °C.

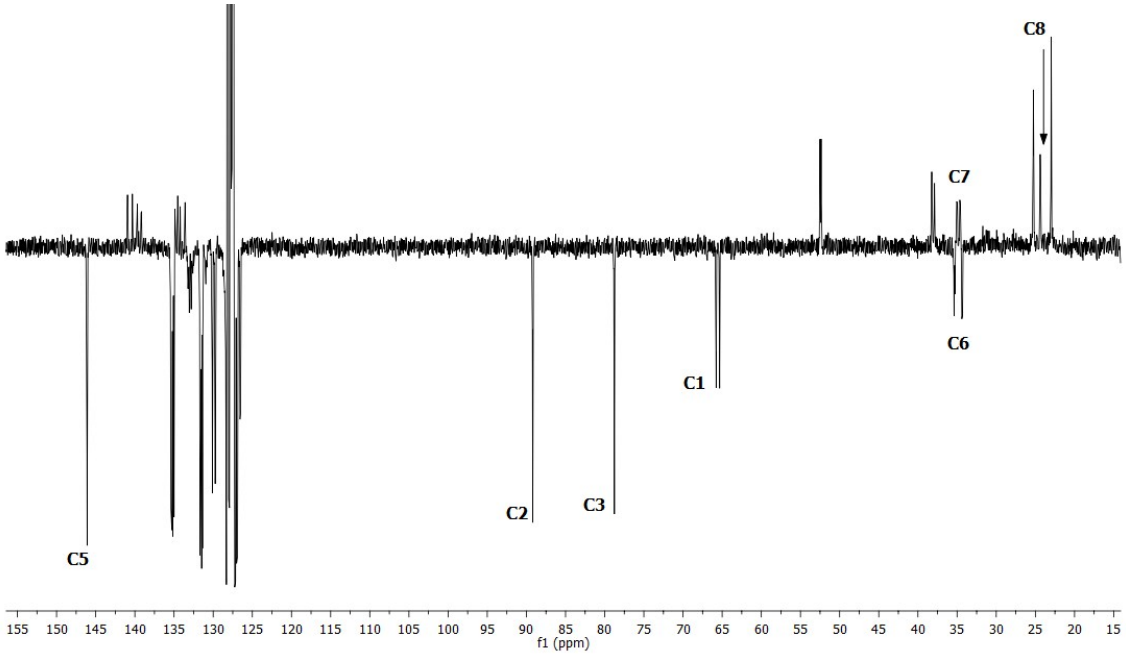


Figure S9. ^{1}H-^{31}P HMBC NMR spectrum of **6** in C_6D_6 at 25 ^{o}C.

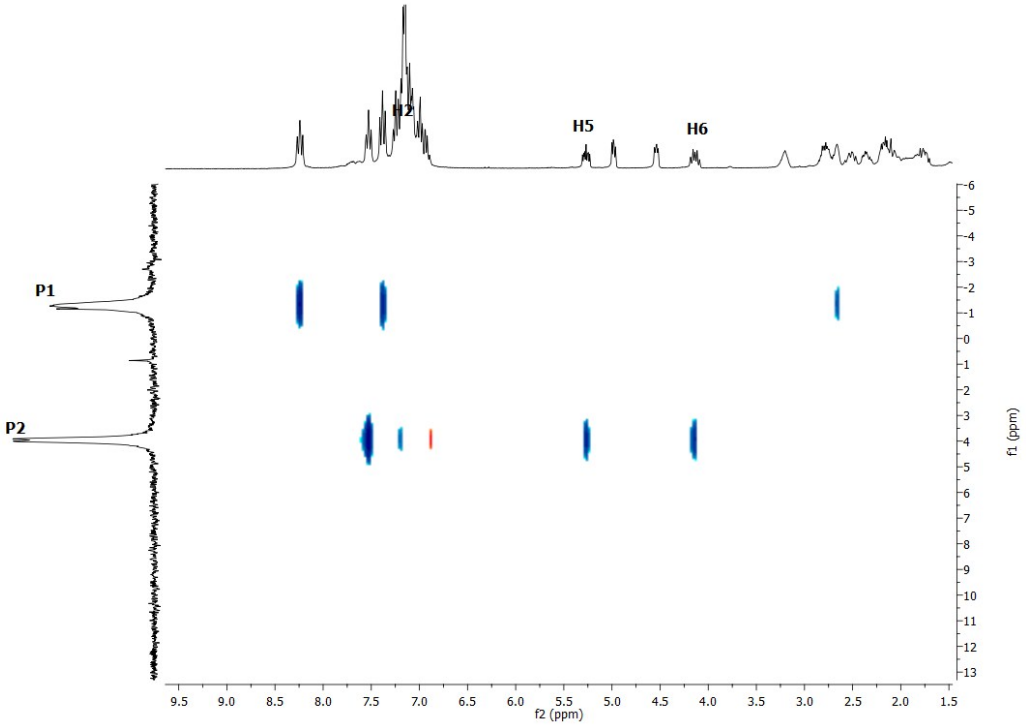


Figure S10. Selected region of the ^{1}H-^{13}C HSQC NMR spectrum of **5** in C_6D_6 at 25 ^{o}C.

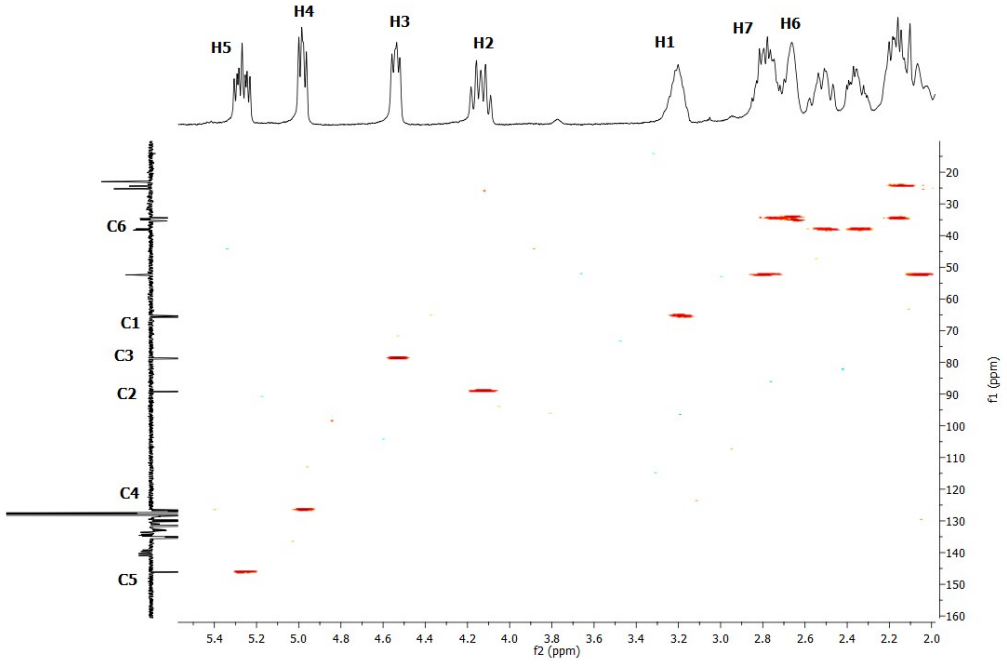


Figure S11. ^{1}H NMR spectrum of **6** in CD_2Cl_2 at –50 °C.

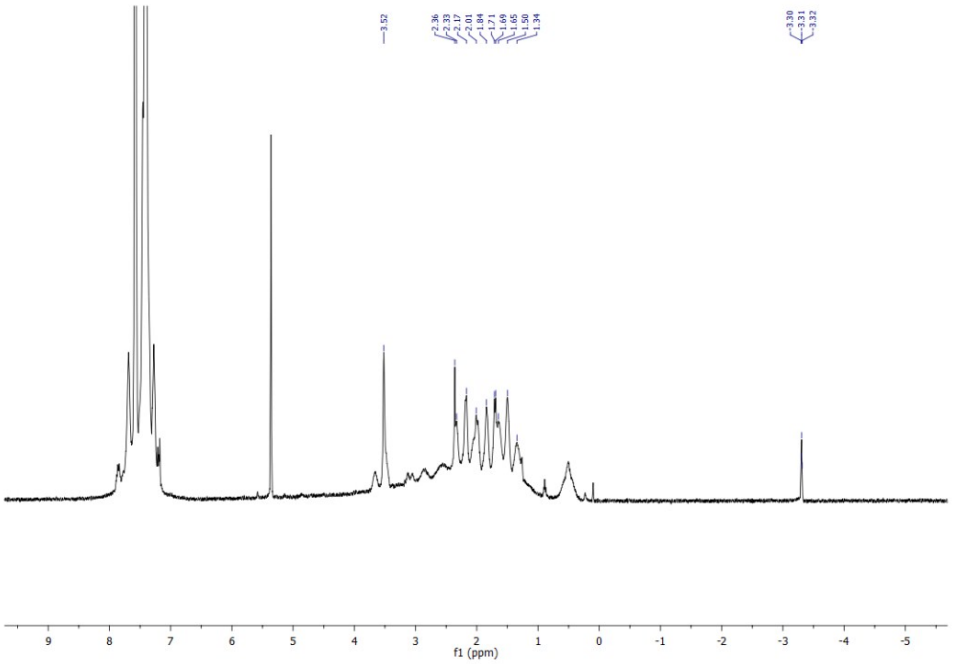


Figure S12. $^{31}P\{^{1}H\}$ NMR spectrum of **6** in CD_2Cl_2 at –50 °C.

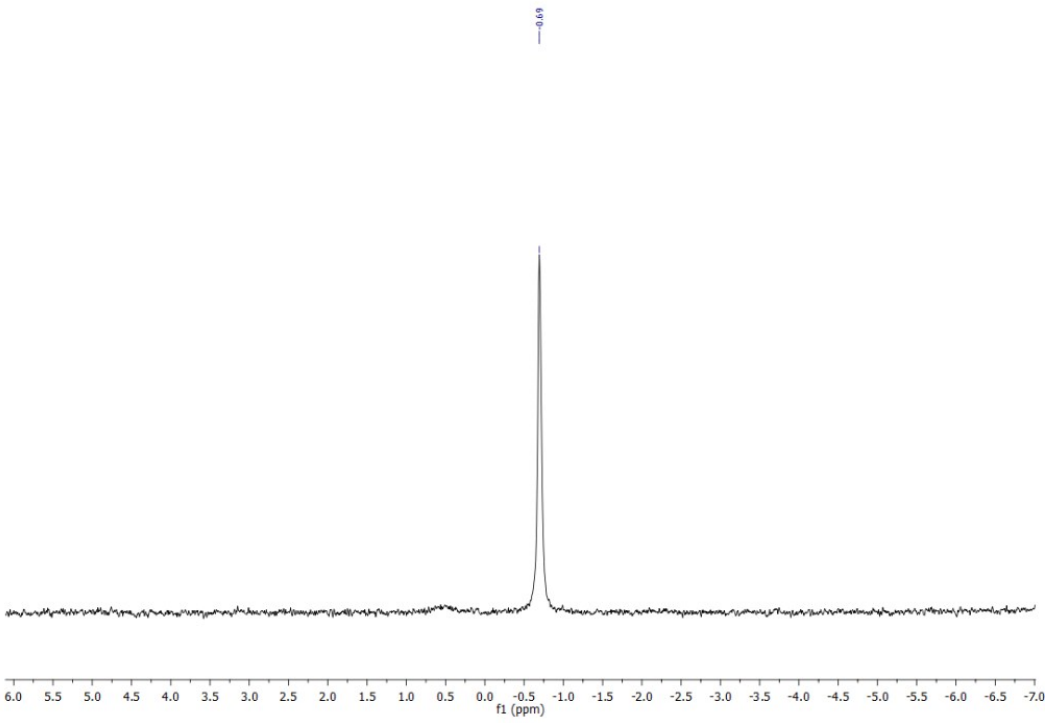


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of **6** in CD_2Cl_2 at −50 °C.

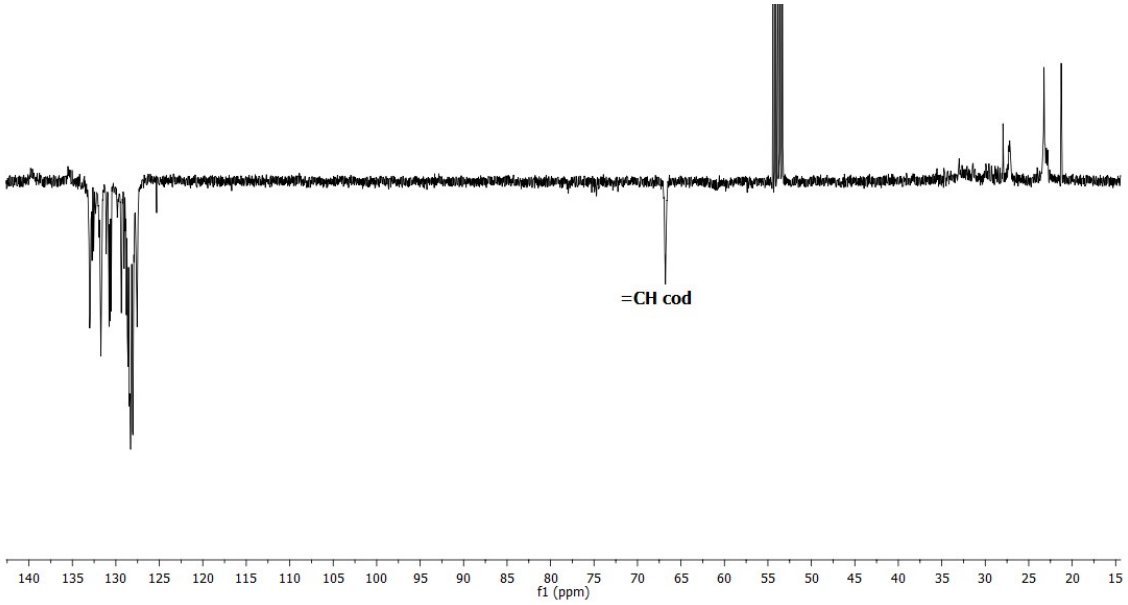


Figure S14. ^{1}H NMR spectrum of **7** in C_6D_6 at 0 °C.

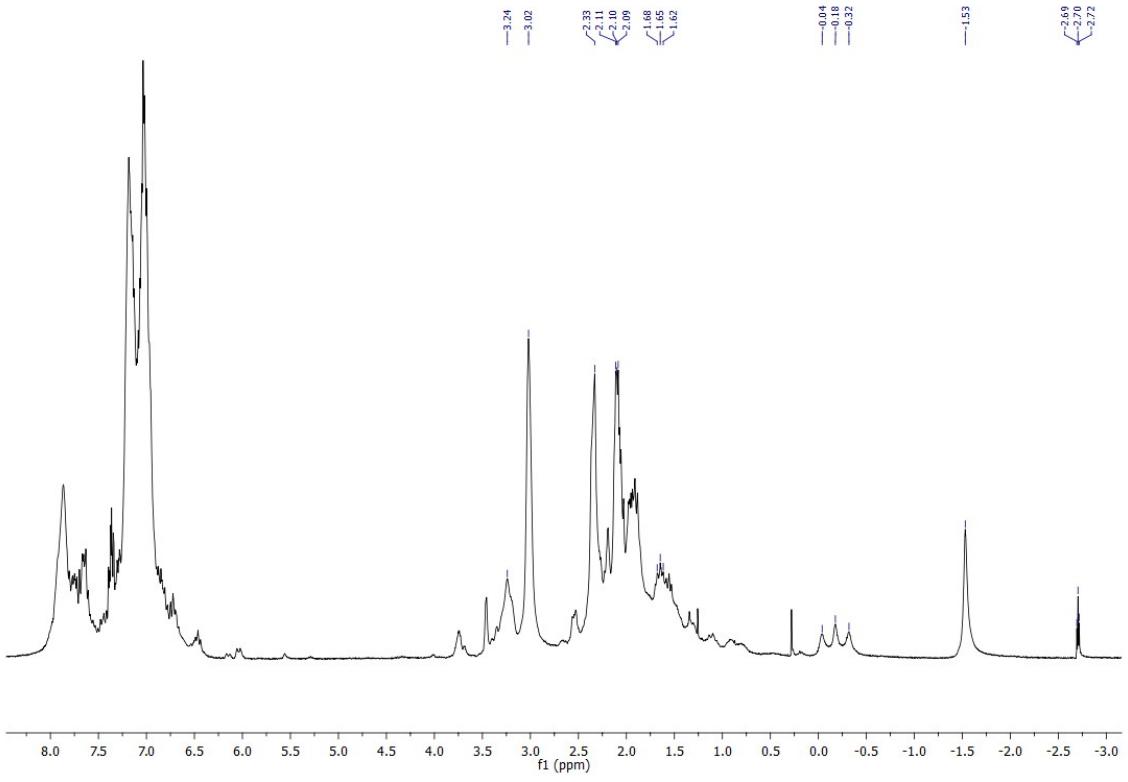


Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum of **7** in C_6D_6 at 0 ^{o}C.

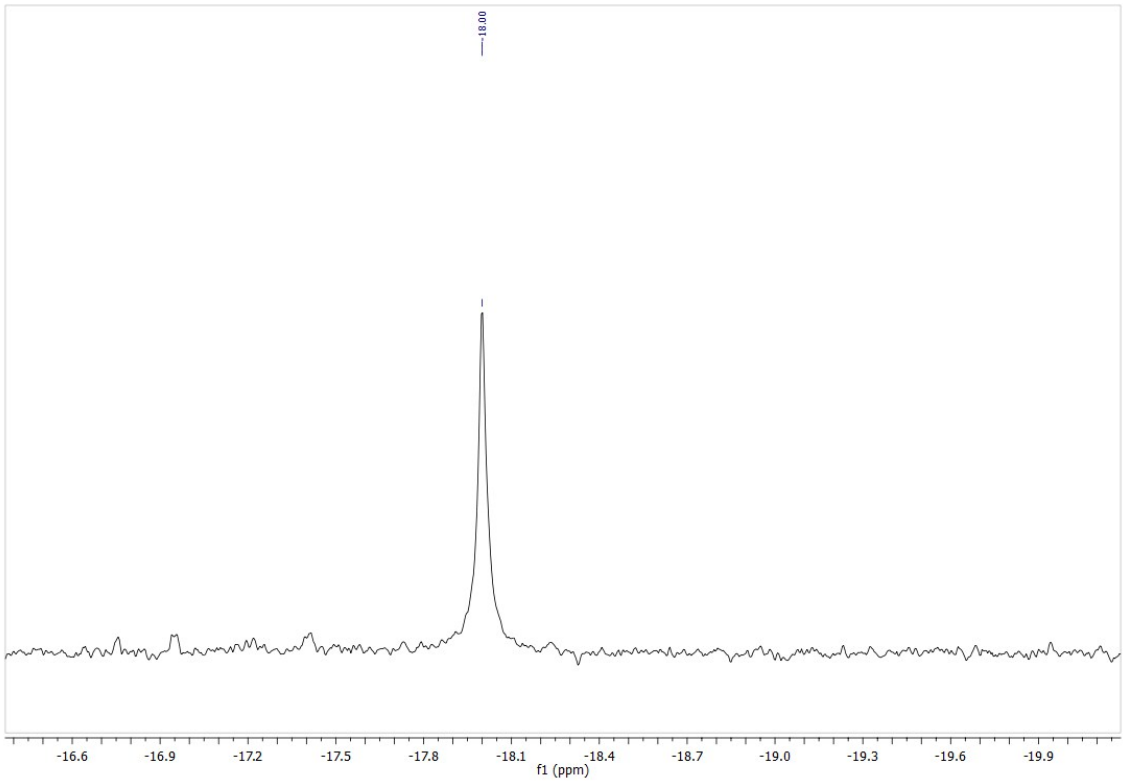
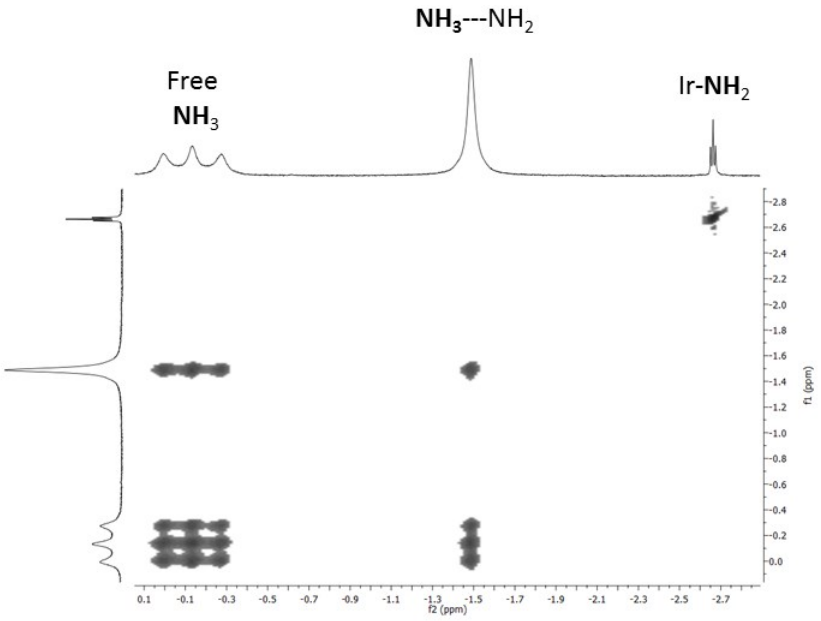


Figure S16. Detail of the ^{1}H-^{1}H NOESY spectrum of **7** in C_6D_6 at 0 ^{o}C.

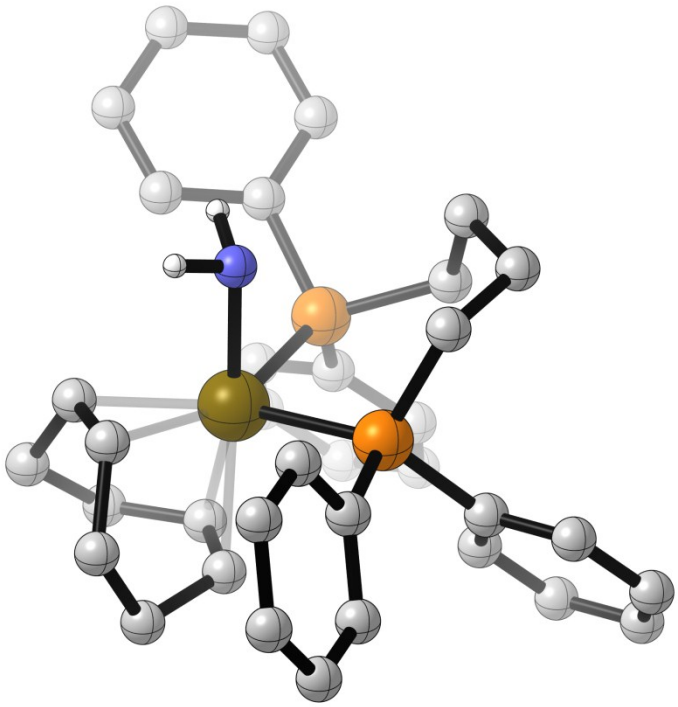


Computational data

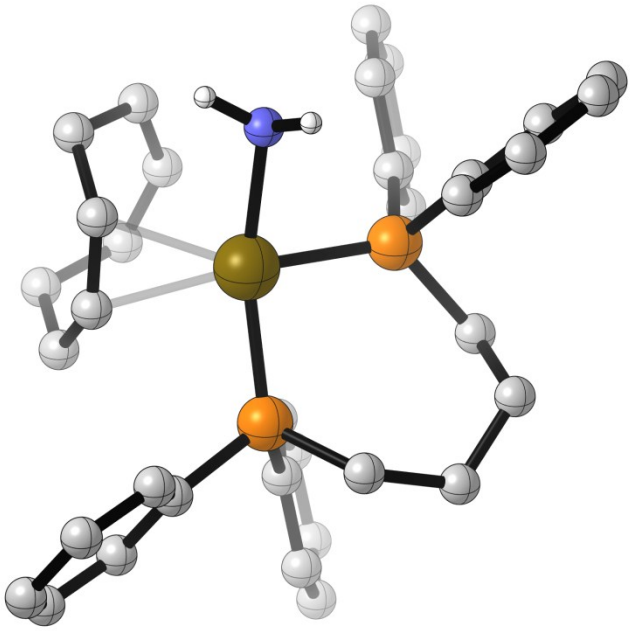
Table S1. Energetic values for DFT calculated structures. Geometrical optimizations using the def2-SVP, E(DZ), basis set and single point energies using solvent corrections at the PCM level and def2-TZVP basis set E(TZ,PCM). Correction to the Gibbs free energy 25 ºC in a 1 atm standard state calculated at the def2-SVP level, G(DZ). All absolute energies in a.u. Gibbs free energies relative to **A** and isolated molecules considering solvent and triple-Z corrections in kcal mol^{-1}.

	E(DZ)	G(DZ)	E(TZ,PCM)	G(TZ,PCM)	DG(TZ,PCM)
A	−2238.04522	0.62423	−2239.86681	−2239.24258	0.0
A'	−2238.00897	0.62158	−2239.83511	−2239.21354	18.2
TSA'C	−2237.99612	0.61211	−2239.81927	−2239.20716	22.2
C	−2238.01209	0.62070	−2239.83754	−2239.21684	16.2
D	−2181.50177	0.58287	−2183.26014	−2182.67726	−4.9
TSDE	−2181.46285	0.57852	−2183.22110	−2182.64258	16.8
E	−2181.51055	0.58407	−2183.26992	−2182.68586	−10.3
TSAB	−2237.97580	0.61326	−2239.80257	−2239.18931	33.4
B	−2238.01322	0.62151	−2239.83456	−2239.21305	18.5
TSBC	−2237.97832	0.61886	−2239.80134	−2239.18248	37.7
NH_3	−56.51070	0.01600	−56.58919	−56.57319	

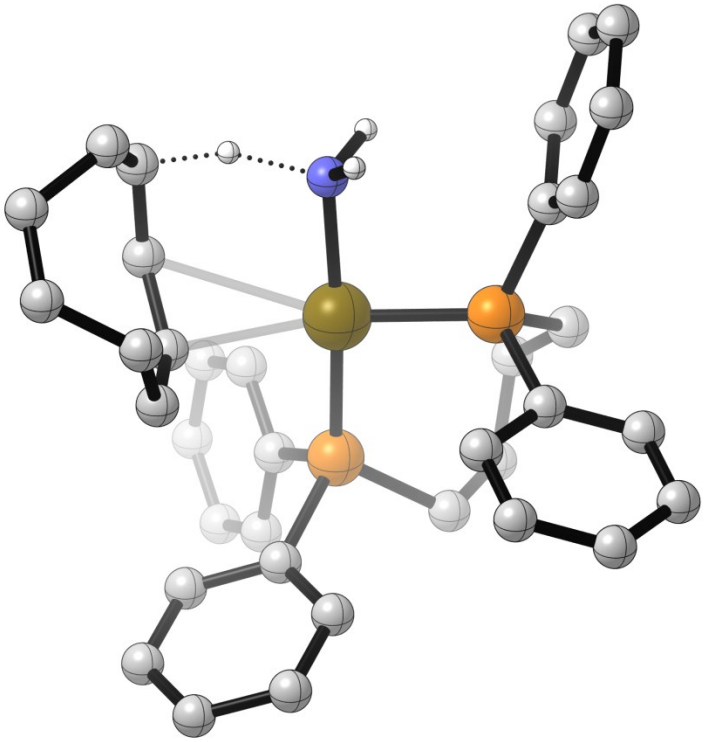
Figure S17. Geometrical representation of all DFT calculated structures. Hydrogen atoms bonded to carbon atoms are omitted for clarity.



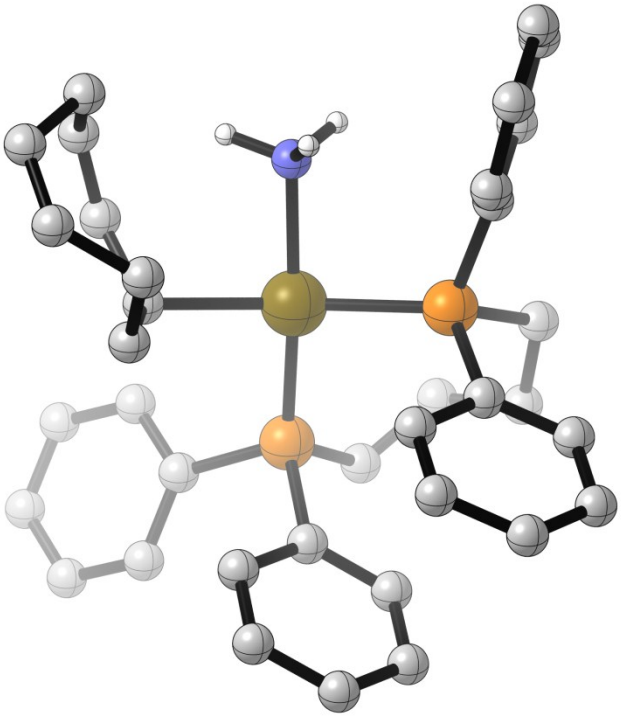
A



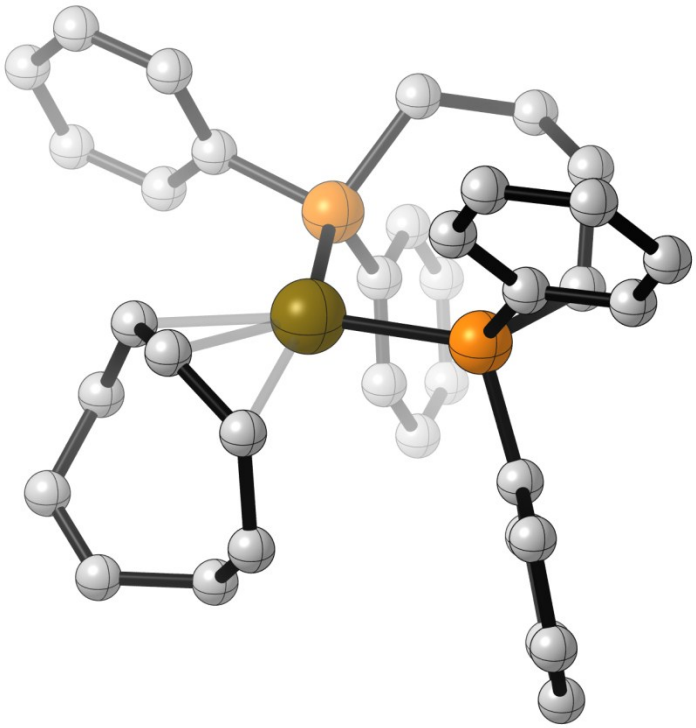
A'



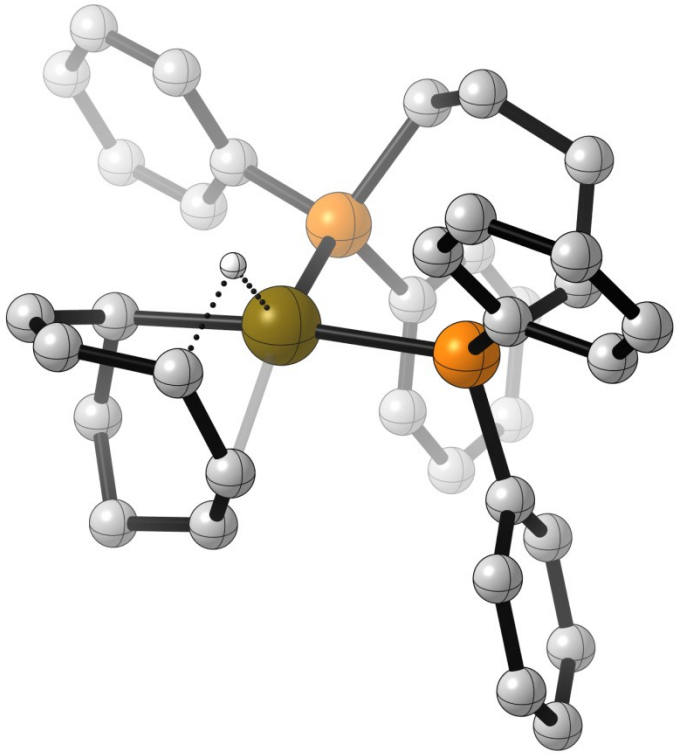
TSA'C



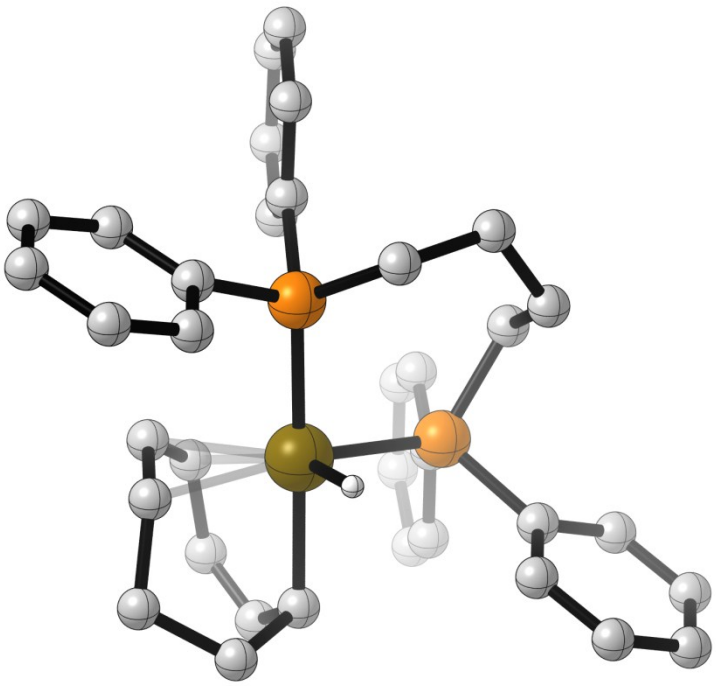
C



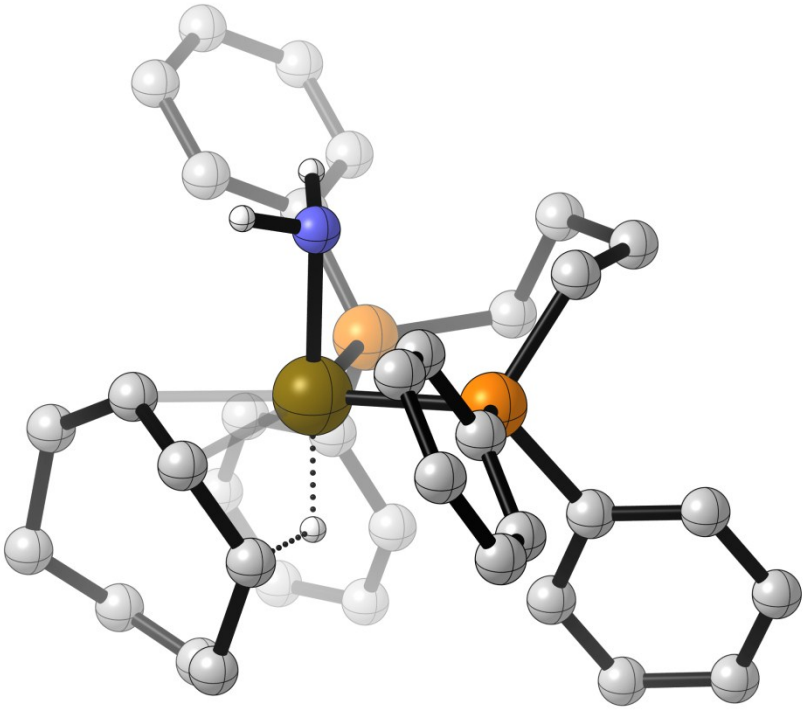
D



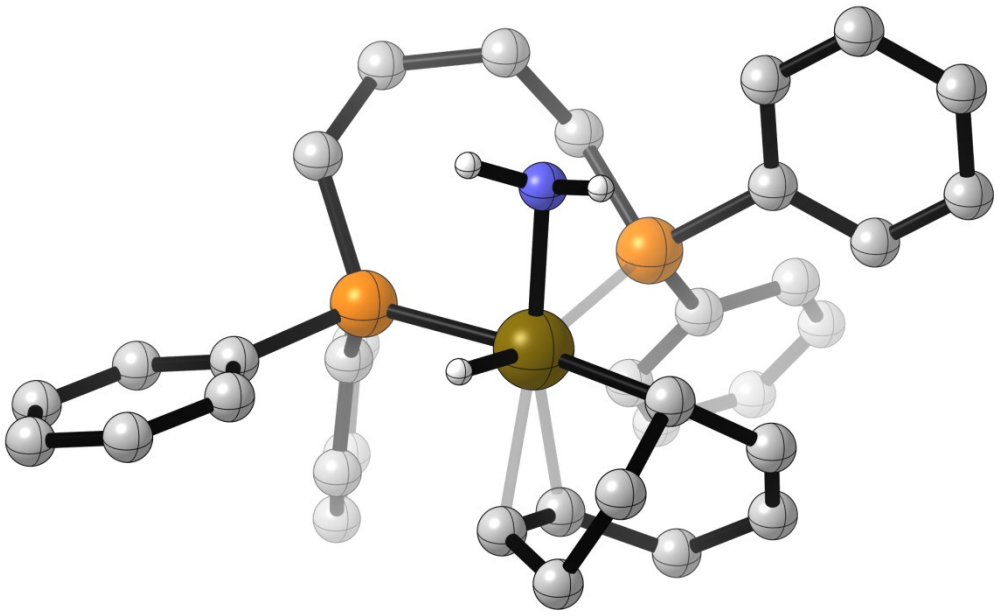
TSDE



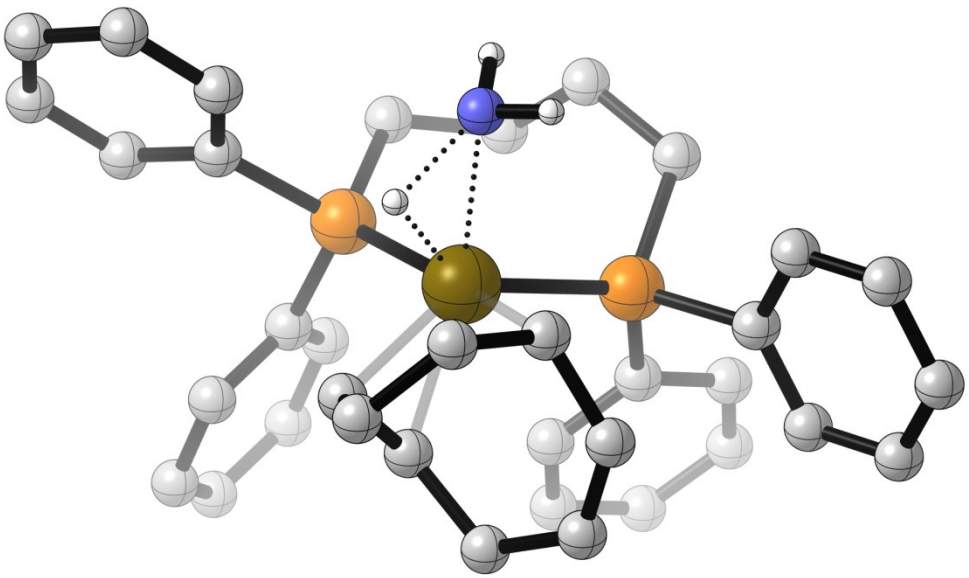
E



TSAB



B



TSBC

Table S2. Cartesian coordinates (in Å) for all DFT calculated structures:

A

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A’

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TSA'C

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