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SUPPLEMENTARY INFORMATION

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A hexagonal planar transition-metal complex

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Supporting Information for:

A Hexagonal Planar Transition Metal Complex

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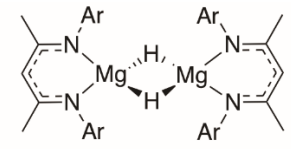
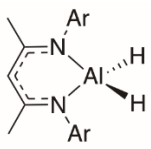
1. Experimental details

Unless otherwise specified, all manipulations were carried out using standard Schlenk and glovebox techniques, under inert atmosphere (nitrogen or argon). A MBRAUN Labmaster glovebox was employed operating with concentrations of H_2O and O_2 below 0.1 ppm. Anhydrous solvents were obtained from a Grubbs type SPS system and stored over activated 3Å molecular sieves under inert atmosphere. Alternatively, they were dried using molecular sieves and degassed by freeze-pump-thaw procedures. Stable liquid organic reagents were dried over 3Å molecular sieves and freeze-pump-thaw degassed before use. All other reagents were obtained from commercial suppliers (Sigma-Aldrich, Alfa Aesar, Fluorochem) and used without further purification. ^{Dipp}BDIH,[1] ^{Mes}BDIH,[2] $Me_3N{\cdot}AlH_3$,[3] [^{Dipp}BDIMg(μ-H)]$_2$ (**S1**),[4] ^{Dipp}BDIAlH$_2$ (**S2**),[5] and ^{Mes}BDIMg–MgBDI^{Mes} (**S3**)[6] were prepared by literature procedures (^{Dipp}BDI = {2,6-i-Pr$_2$C$_6$H$_3$NC(Me)}$_2$CH, ^{Mes}BDI = {2,4,6-Me$_3$C$_6$H$_2$NC(Me)}$_2$CH). [Pd(Me)$_2$(κ^2-TMEDA)],[7] [Pd(η^5-Cp)(η^3-cinnamyl)],[8,9] were synthesised by literature methods as was [Pd(PCy$_3$)$_2$] due to the insufficient purity of commercial samples.[9] [Pt(PCy$_3$)$_2$] was synthesised by modified literature procedures, as detailed below.



S1
Ar = 2,6-di-iso-propylphenyl



S2
Ar = 2,6-di-iso-propylphenyl

S3
Ar = Mes

^{1}H-, ^{13}C-, ^{31}P- and ^{195}Pt-NMR spectra and two-dimensional experiments (COSY, NOESY, DOSY, HSQC, HMBC, ^{1}H-^{31}P-HMBC) were conducted in J. Young's NMR tubes on BRUKER 400 MHz or 500 MHz spectrometers. Chemical shifts (δ) were referenced to internal solvent resonances. Data was processed using the MestReNova or TopSpin software. The coupling constants (*J*) are reported in Hertz (Hz). The following abbreviations are used to define multiplicities: s (singlet), d (doublet), t (triplet), q (quadruplet), sept. (septet), dd (doublet of doublets), m (multiplet), br s (broad signal).

In order to better study some of the equilibrium processes, a quantitative ^{31}P-{^{1}H}-NMR experiment was used. Inverse-gated ^{1}H decoupling was used to suppress NOE. PPh_3 in C_6D_6 was used as the internal standard and the T_1 relaxation times of the ^{31}P signals were measured to ensure full relaxation of the signals. The experiments were set with 80 scans and a delay of 130s.

Single crystal X-Ray data was obtained on Agilent Diffraction Xcalibur PX Ultra A and Xcalibur 3 E diffractometers, and the structures were refined using the SHELXTL and SHELX-2013 program systems.[10]

Neutron Laue data were collected on the KOALA instrument at the Australian Nuclear Science and Technology Organization (ANSTO). A total of 102818 reflections with wavelengths between 0.85 and 1.70 Å covering the full sphere of reciprocal space to a maximum resolution of 0.98 Å were reduced to yield 8847 independent reflections [L4R(int) = 0.10(7)]; 4816 with $I > 3\sigma(I)$. Data were collected from a yellow single-crystal (1.0 x 1.0 x 1.8 mm^3) mounted to the phi axis of the KOALA diffractometer which stands at an end position of TG3 - a supermirror thermal neutron guide at the OPAL nuclear reactor at ANSTO. A total 53 Laue diffraction images (55 minutes per exposure) were collected with rotation of the crystal around the phi axis occurring between exposures. Owing to the triclinic space group, data were collected from two orientations of the crystal to complete coverage of reciprocal space. Data reduction was by means of the LAUEG suite.[11,12]

The unit-cell is as for the X-ray determination as it cannot be reliably determined using Laue neutron diffraction – related data such as space group are the same. Care was taken to ensure that the temperature of the experiment was matched to the X-ray experiment using an Oxford Cryosystems COBRA™ cryostream which also served to protect the crystal from moisture and oxygen, the sample was handled immersed in argon to ensure compound stability while the crystal was transferred to the coldstream.

2. Preparation of Starting Materials

2.1 Synthesis of [Pt(PCy$_3$)$_2$]

A known procedure was modified.[13] A Schlenk flask was charged with K_2PtCl_4 (500 mg, 1.2 mmol, 1 equiv.), deoxygenated water (2.5 mL), and an ethanol solution (25 mL) of PCy_3 (750 mg, 2.67 mmol, 2.2 equiv.). The mixture was stirred at 25°C for 15h and a colourless solid slowly precipitated. The solid was filtered under air, washed successively with water (20 mL) and ethanol (20 mL), and dried under reduced pressure. *trans*-[$PtCl_2(PCy_3)_2$] was isolated as a white solid (320 mg, 0.39 mmol, 32%).

trans-[$PtCl_2(PCy_3)_2$] was used without further purification. A 1% sodium amalgam was prepared in a Schlenk flask by slowly adding Na pieces (17.5 mg, 0.76 mmol, 2.1 equiv.) to Hg (14.6 g, 72.6 mmol, 200 equiv.). [$PtCl_2(PCy_3)_2$] (300 mg, 0.36 mmol, 1 equiv.) was suspended in dry THF and then added to the freshly prepared Na(Hg). The mixture was heated to 55-60°C for two days with vigorous stirring. The mixture was then allowed to cool down to 25°C and filtered *via* cannula. The THF was evaporated under reduce pressure and the crude solid extracted with hot *n*-hexane (20 mL x2). The *n*-hexane was then removed *in vacuo* until crystallisation of the product began. The mixture was left at -35°C to induce further crystallisation. The solid was isolated by filtration and dried under vacuum. The solid was taken into the glovebox, where it was washed with *n*-hexane (1 mL x2) and dried *in vacuo* to afford the [$Pt(PCy_3)_2$] as a pale brown solid (194 mg, 0.26 mmol, 71%).

^{1}H-NMR (400 MHz, C_6D_6) δ (ppm): 1.18–1.33 (m, 9H), 1.58–2.03 (series of overlapping m, 18H), 2.23–2.34 (m, 6H).

^{31}P-{^{1}H}-NMR (162 MHz, C_6D_6) δ (ppm): 62.10 (s, $^1J_{P\text{-}Pt}$ = 4163 Hz – satellites).

Data are consistent with those previously reported.[13]

3. Solution NMR Data: Equilibrium Studies

Most of the reported complexes undergo H/D exchange in the transition metal hydride positions if the reactions are performed in C_6D_6 instead of C_6H_6.

3.1 Multinuclear NMR data for 2a and 2b

Figure S1. The solution equilibria of **2a** and **2b**.

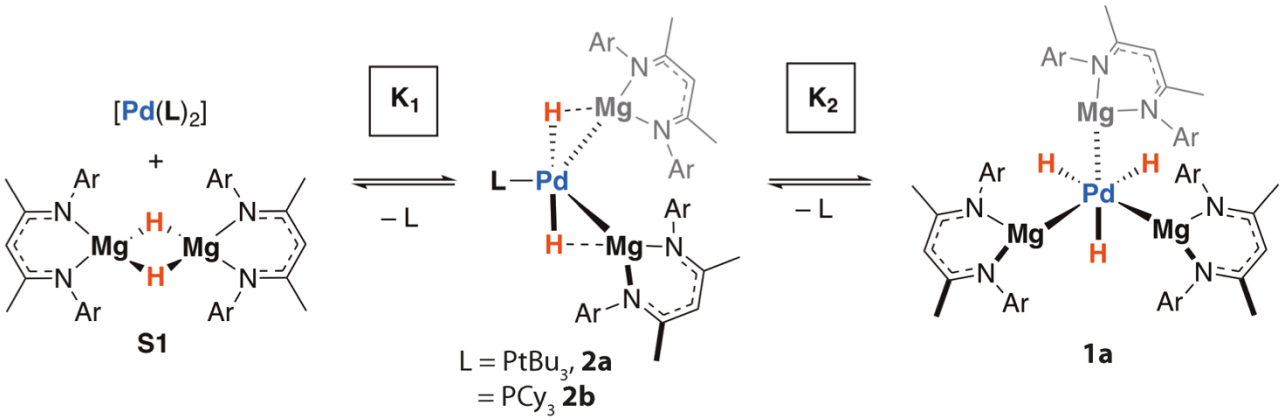


Figure S2. VT of the ^{31}P-NMR of **2b** in toluene-d^8 showing the shift of the equilibrium toward **2b** and the formation of [Pd(PCy$_3$)$_3$] at lower temperatures.[14]

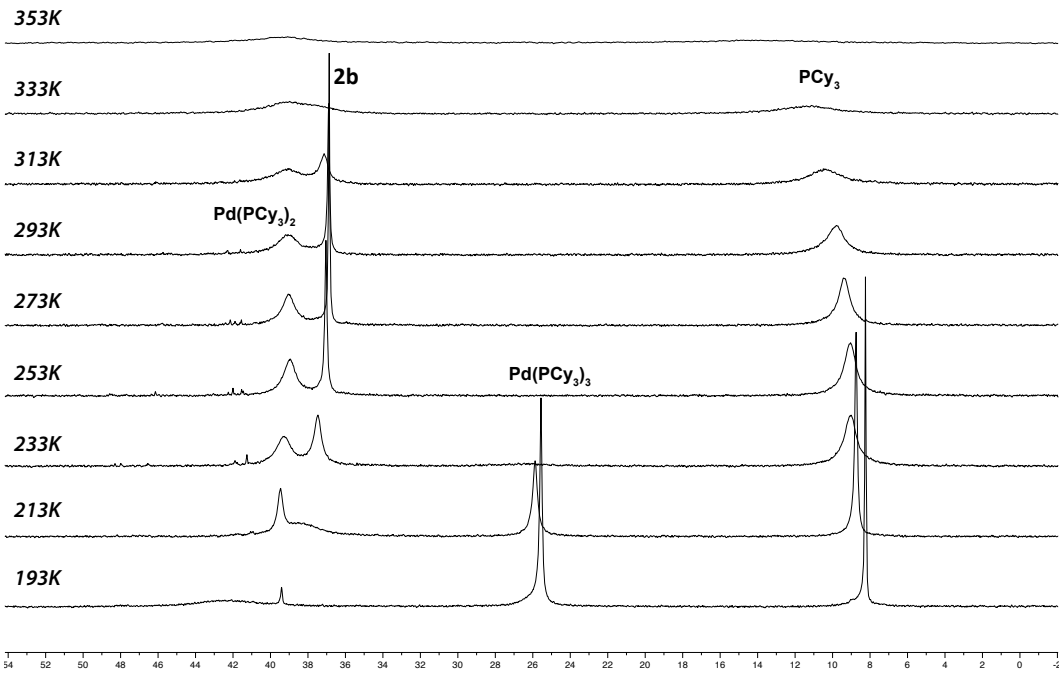


Figure S3. $^{1}H–^{31}P$ HMBC NMR of an equilibrium mixture containing **2b**.

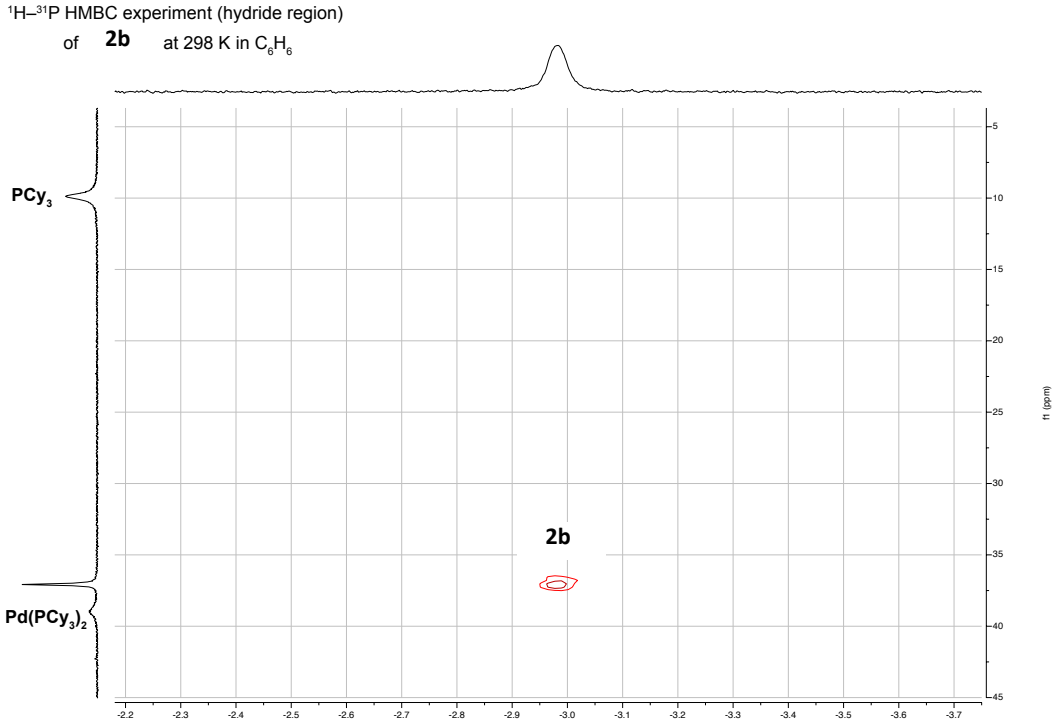


Figure S4. VT of the ^{1}H-NMR of an equilibrium mixture containing **2b** in toluene-d^8 showing the shift of the equilibrium toward **2b** at lower temperatures.

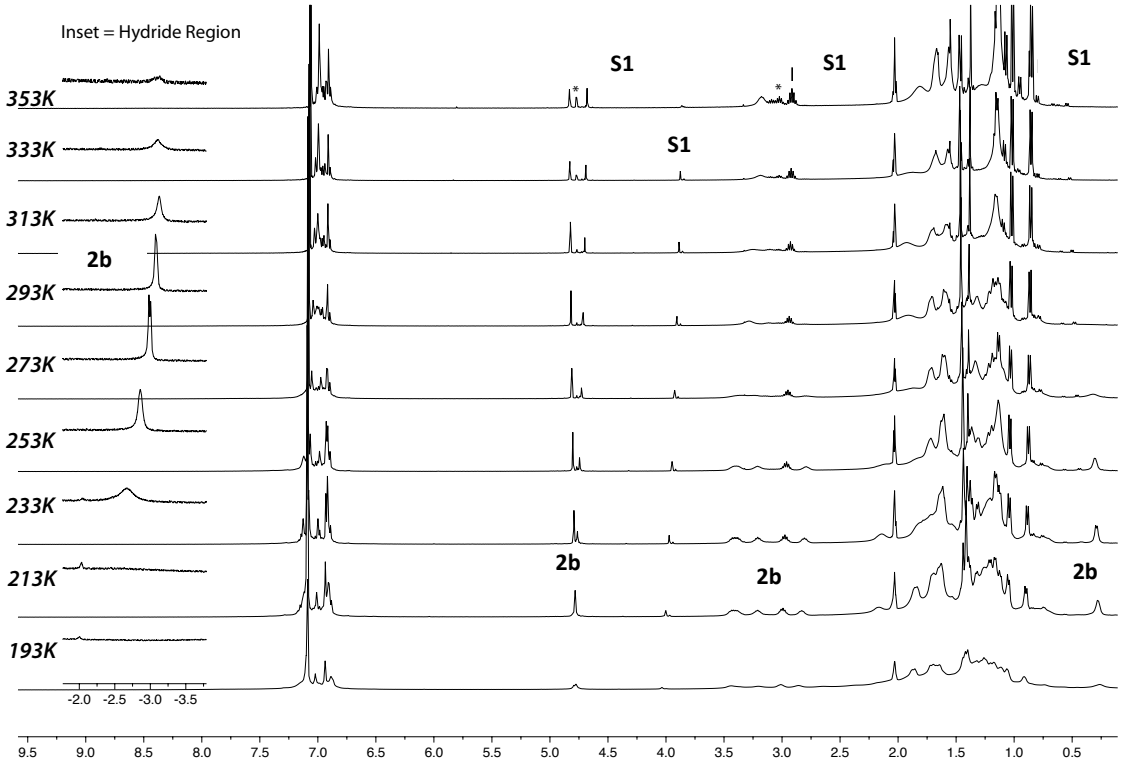


Figure S5. ^{1}H-NMR and ^{1}H-{^{31}P}-NMR of an equilibrium mixture containing **2b** in C_6H_6, at 298K and 283K, showing resolution of $^{2}J_{P-H}$ coupling at 283 K.

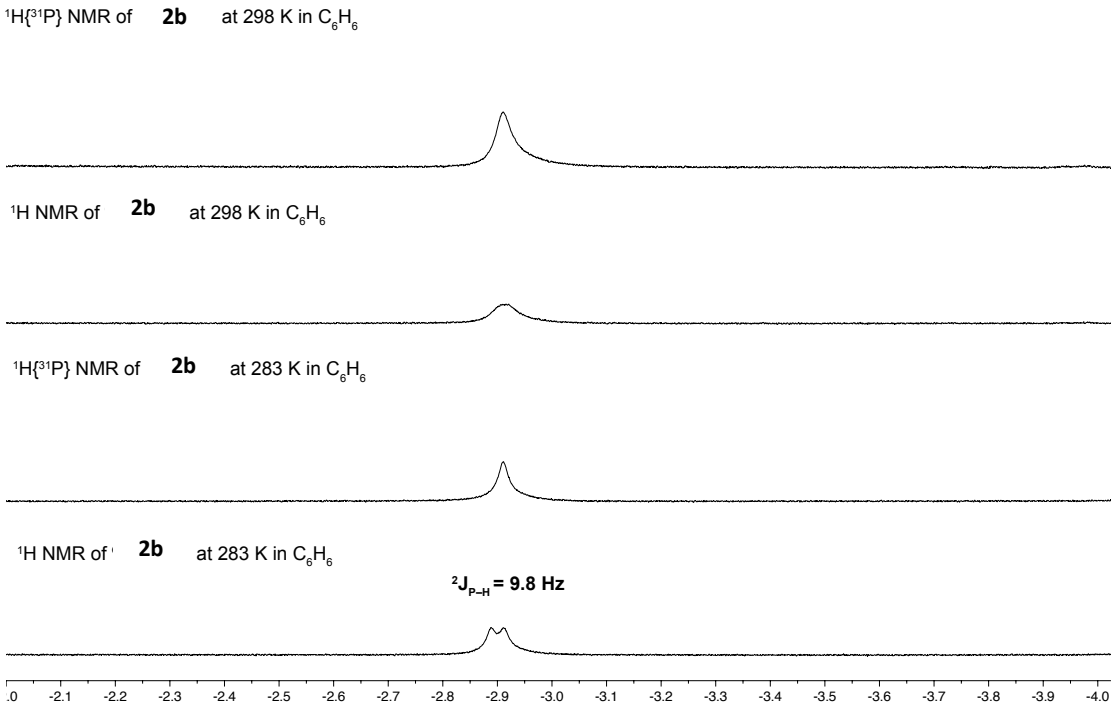
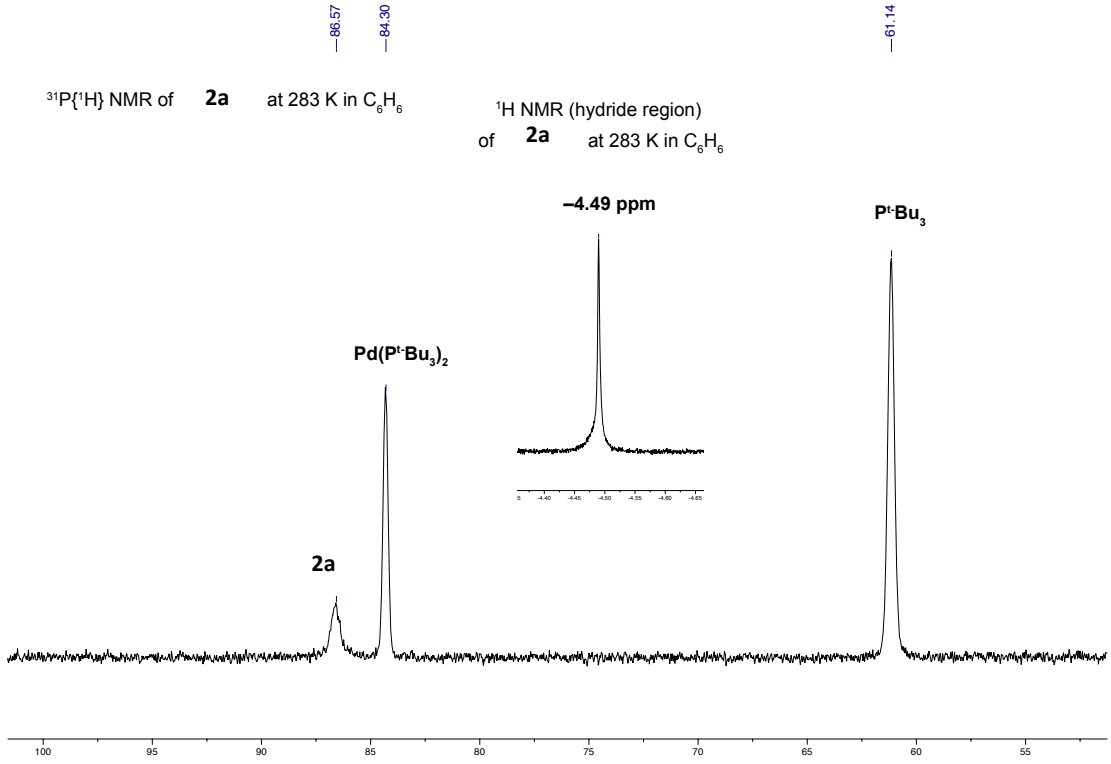


Figure S6. ^{31}P-NMR of an equilibrium mixture containing **2a** with insert of hydride region of the ^{1}H-NMR spectrum at 283 K in C_6H_6.



3.2 Quantification of the equilibrium data for 2b

In order to further characterise the whole equilibrium, a NMR titration was performed. A known concentration of **S1** was titrated with increasing amounts of [Pd(PCy_3)$_2$]. Monitoring the concentrations of **S1**, **1a** and **2b**, an approximate ratio of the equilibrium constants K_2/K_1 could be obtained.

$$K_1 = \frac{[2b][PCy_3]}{[Pd(PCy_3)_2][S1]^2} \qquad (1)$$

$$K_2 = \frac{[1a][PCy_3]}{[2b][S1]} \qquad (2)$$

$$\frac{K_2}{K_1} = \frac{[1a][Pd(PCy_3)_2][S1]}{[2b]^2} \qquad (3)$$

At equilibrium, the total concentration of Pd equals the sum of the concentration of all Pd containing species, which is also equal to the initial concentration of added [$Pd(PCy_3)_2$].

$$[Pd(PCy_3)_2]_i = [Pd]_{total} = [Pd(PCy_3)_2] + [1a] + [2b] \qquad (4)$$

And thus, substituting [$Pd(PCy_3)_2$] into equation (3), we obtain the following expression,

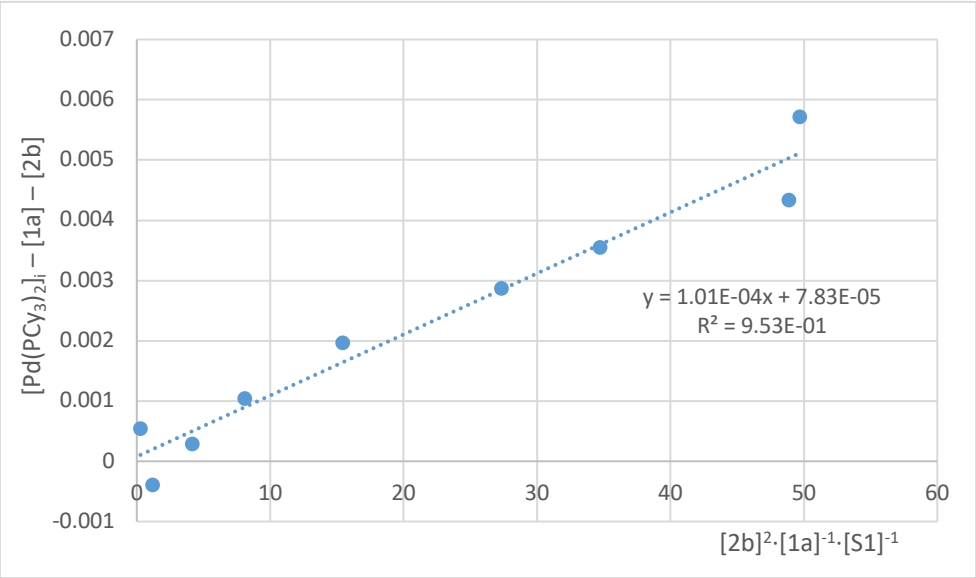
$$\frac{K_2}{K_1} \cdot \frac{[2b]^2}{[1a][S1]} = [Pd(PCy_3)_2]_i - [1a] - [2b] \qquad (5)$$

As such, plotting $\{[2b]^2 \cdot [1a]^{-1} \cdot [S1]^{-1}\}$ vs $\{[Pd(PCy_3)_2]_i - [1a] - [2b]\}$ at every point of the titration will provide a line of slope = K_2/K_1.

Table S1: NMR titration of **S1** with $Pd(PCy_3)_2$. Concentrations in M.

Point	Equiv. of $Pd(PCy_3)_2$	[S1]	[2b]	[1a]	$[Pd(PCy_3)_2]_i$	V total (mL)
0	0.0	0.0168	0.0000	0.00000	0.0000	0.50
1	0.1	0.0123	0.0005	0.00008	0.0011	0.53
2	0.2	0.0148	0.0023	0.00029	0.0021	0.56
3	0.3	0.0096	0.0026	0.00017	0.0031	0.59
4	0.5	0.0055	0.0033	0.00025	0.0046	0.65
5	0.7	0.0040	0.0037	0.00023	0.0059	0.71
6	0.9	0.0027	0.0039	0.00021	0.0070	0.77
7	1.0	0.0020	0.0038	0.00020	0.0075	0.80
8	1.2	0.0019	0.0039	0.00016	0.0084	0.86
9	1.5	0.0018	0.0036	0.00015	0.0095	0.95

Figure S7. Plot of the NMR titration data to obtain the relationship between equilibrium constants (slope = K_2/K_1).



As expected, K_2 was found to be significantly smaller than K_1 ($K_2/K_1 = 10^{-4}$), which is consistent with the fact that only very small amounts of **1a** are present in the equilibrium mixture.

3.3 Equilibrium Data for 3

The solution behaviour of **3** is quite complex. **3** has minimal solubility in apolar organic solvents such as *n*-hexane and benzene. It is more soluble in polar organic solvents such as THF, although the complex will degrade on the hour time scale. Full NMR characterization could be achieved in THF-d_8 at 273 K, with no degradation observed over a 6 h period. Analysis of the NMR spectra in benzene-d_6 (sonicated in benzene-d_6, no heating: minimal solubility) revealed small amounts of complex **3**, with hydride signals located at -7.04 ppm. After standing at 298 K overnight, these hydride signals had been washed out by H/D exchange with the deuterated solvent.[i] A second set of peaks were observed in the ^{1}H NMR spectrum. Concomitantly, if **3** is heated in a solution of benzene-d_6, the complex dissolves and a colour change occurs from yellow to orange (back to yellow upon cooling). NMR analysis reveals the presence of two species (as above), one containing bound phosphine (**3**) and one with no bound phosphine postulated to be **1c** (free PCy_3 was observed in the $^{31}P\{^1H\}$ NMR). Variable temperature NMR studies (see section 4) show that as the solution is heated to 80 °C, the equilibrium is affected, and the mixture exists exclusively as **1c** and free phosphine (orange solution observed at high temperature). The solution stability of **1c** and **3** in apolar organic solvents is poor, and the compound degrades over the course of a couple of days. The equilibrium mixture readily crystallises as **3**, to date no crystals of **1c** have been isolated.

[i] The hydride ligands are presumed to originate from the C–H activation of the solvent. We have previously shown that a closely related Ni system is catalytically active for the C–H activation of benzene with **S3** (*Chem. Commun.* **2018**, *54*, 12326).

Figure S8. The proposed solution equilibria of **3**.

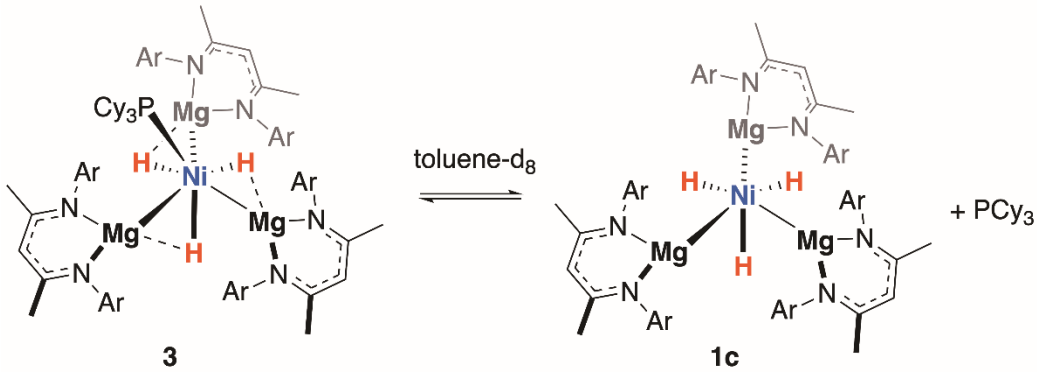


Figure S9. VT of the $^{31}P\{^{1}H\}$-NMR of **3** in toluene-d_8 showing the shift of the equilibrium toward **3** at lower temperatures.

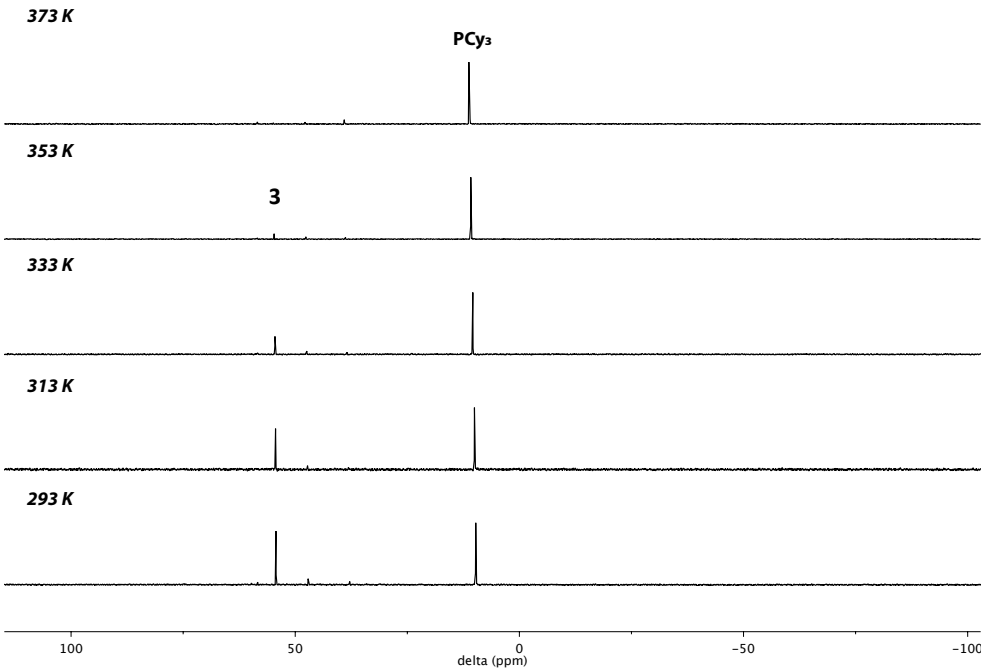
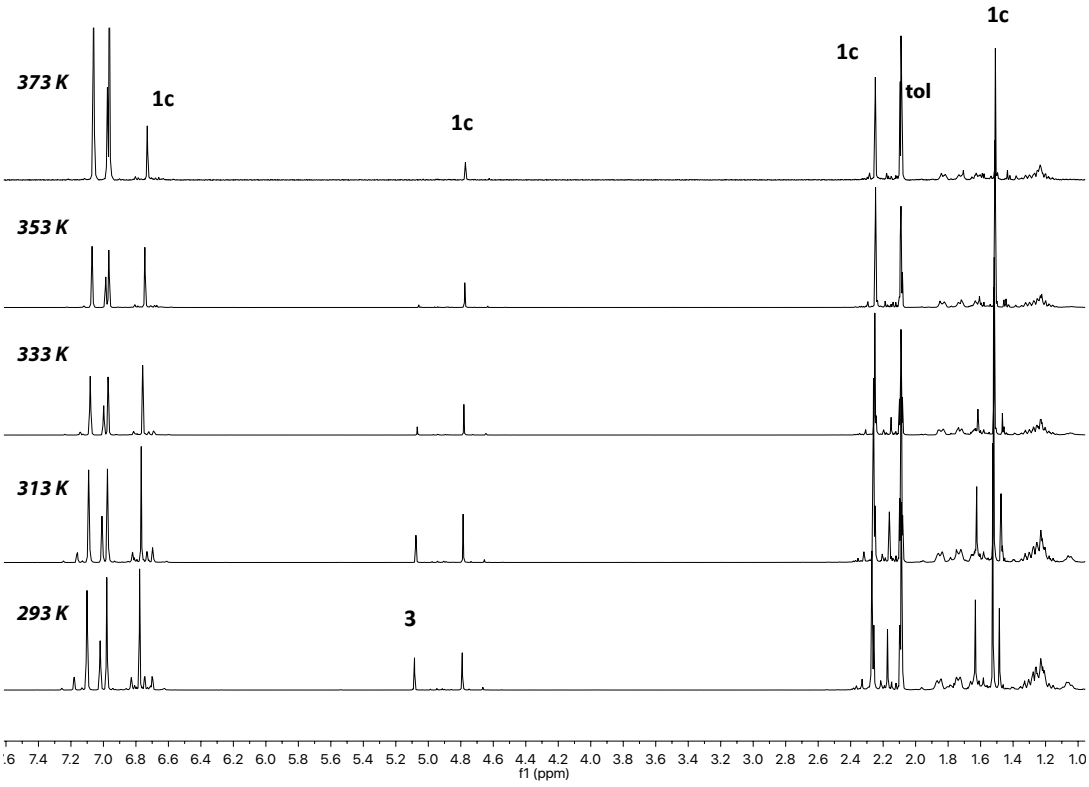


Figure S10. VT of the ^{1}H-NMR of **3** in toluene-d_8 showing the shift of the equilibrium toward **3** at lower temperatures along with the formation of a highly symmetric complex assigned as **1c**.Hydride resonances not observed across this temperature range.



4. Single Crystal Diffraction Studies

Figure S11. **a,** The solid-state structures of **1b** and **2c** along with **b,** selected bond lengths (Å).

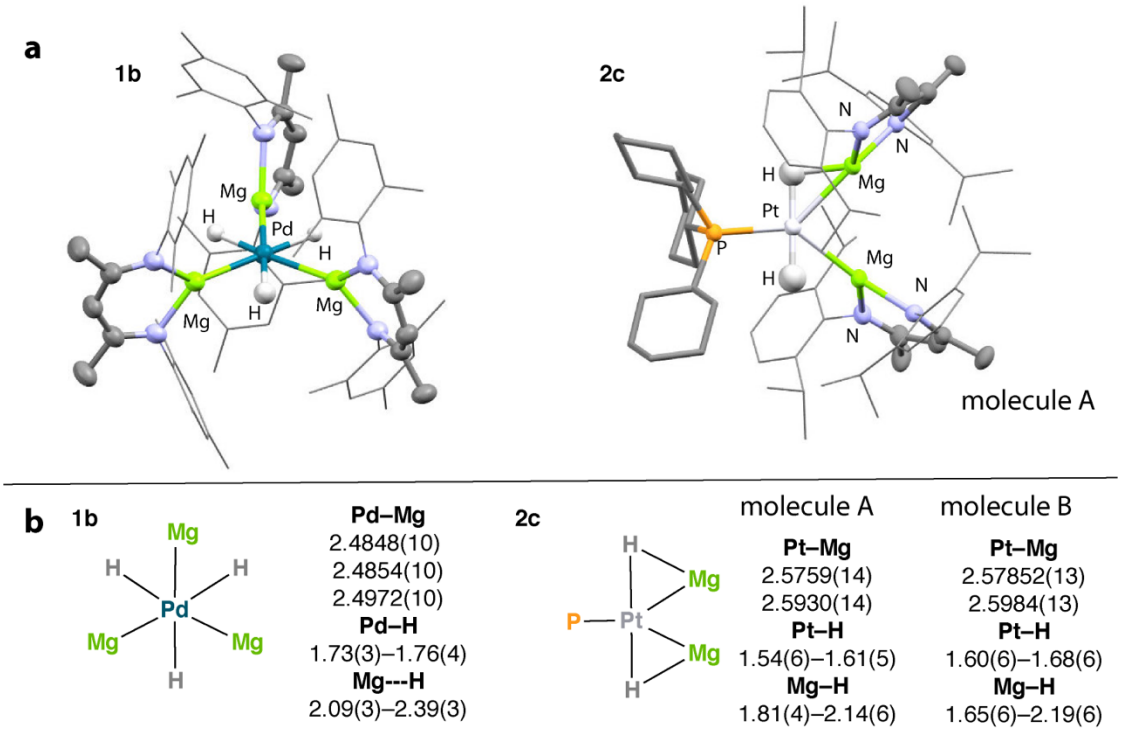
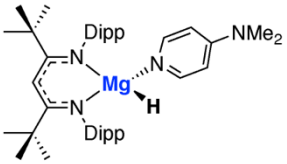


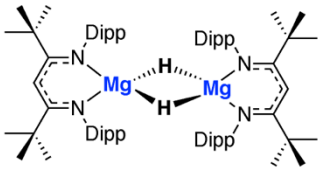
Table S2: Comparison of key metal hydride lengths in **1a, 1b** and **2b** from X-ray diffraction.

Bond length	1a (Å)	1b (Å)	2b (Å)
Pd1–H1	1.58(4)	1.76(4)	1.59(5)
Pd1–H2	1.58(5)	1.73(3)	
Pd1–H3	1.63(4)	1.75(3)	
Mg1–H1	2.43(4)	2.21(3)	1.81(4)
Mg2–H1	2.11(4)	2.15(3)	
Mg2–H2	2.38(4)	2.39(3)	
Mg3–H2	2.21(4)	2.09(3)	
Mg3–H3	2.07(5)	2.28(3)	
Mg1–H3	2.23(4)	2.15(3)	

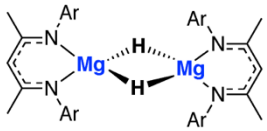
Figure S12. Survey of known β-diketiminate supported magnesium hydride complexes along with X-ray crystallographically determined Mg–H bond lengths.



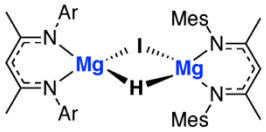
1.75(7) Å
Chem. Eur. J. **2010**, *16*, 938.



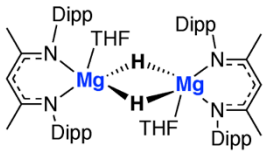
1.80(5) – 1.91(5) Å
Chem. Eur. J. **2010**, *16*, 938.



Ar = Dipp
1.95(3) – 1.97(3) Å
Angew. Chem., Int. Ed. **2008**, 47, 9079.
Chem. Eur. J. **2010**, 16, 8307.



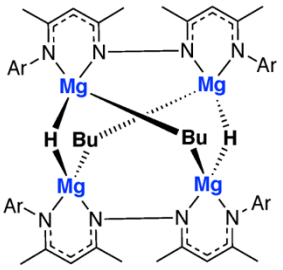
Ar = Dipp
1.88(8) – 1.98(8) Å
Chem. Eur. J. **2010**, *16*, 938.



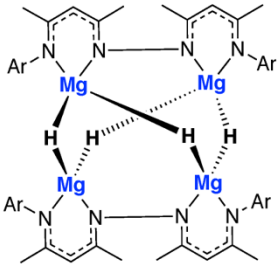
1.95(2) Å
Angew. Chem., Int. Ed. **2008**, *47*, 9079.

Ar = Mes
1.86(2) – 1.89(2) Å
Nat. Chem. **2010**, 865.

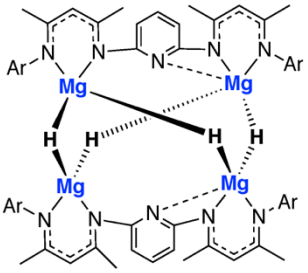
Ar = Dep
1.96(2) – 1.97(2) Å
J. Am. Chem. Soc. **2015**, *137*, 8944.



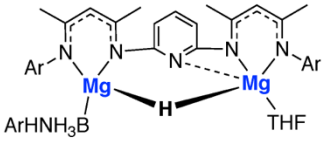
Ar = Dipp
1.76(2) Å
Chem. Eur. J. **2013**, *19*, 8478.



Ar = Dipp
1.77(1) – 1.85(6) Å
Chem. Eur. J. **2013**, *19*, 8478.



Ar = Dipp
1.79(2) – 1.86(2) Å
Dalton Trans. **2014**, 43, 14284.



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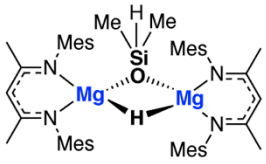
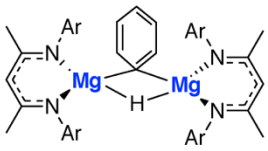
1.93(3) – 1.95(2) Å
Dalton Trans. **2014**, *43*, 14284.

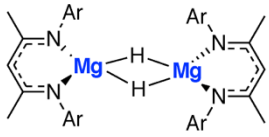


1.85(2) – 1.91(2) Å
Nat. Chem. **2010**, 865.

Ar = Dipp
1.72(3) – 1.90(3) Å
Angew. Chem., Int. Ed. **2011**, *50*, 4156,



Ar = Dipp
1.89(3) – 1.91(3) Å
Chem. Commun. **2018**, *54*, 12326.



Ar = 2,6-di-iso-pentylphenyl
1.96(5) – 1.98(6) Å
Angew. Chem. Int. Ed. **2019**, *58*, 607.

The X-ray crystal structure of 1a

The C57-based isopropyl group in the structure of **1a** was found to be disordered. Two orientations were identified of *ca*. 65 and 35% occupancy, their geometries were optimised, the displacement parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientation were refined isotropically). The C91-based included hexane solvent molecule was found to be disordered across a centre of symmetry. This was modelled using one complete orientation, with a further orientation being generated by operation of the inversion centre. When the unique orientation was refined at the maximum site occupancy of 50%, however, the displacement parameters were too large compared to the rest of the structure (even accounting for the general tendency for disordered solvent molecules to have larger displacement parameters). When refined freely, the occupancy settled at *ca*. 36%, and subsequently it was fixed at exactly 35% for simplicity; all of the non-hydrogen atoms were refined anisotropically. The three Pd–H–Mg bridging hydrogen atoms were all located from Δ*F* maps and refined freely.

The X-ray crystal structure of 1b

The three Pd–H–Mg bridging hydrogen atoms in the structure of **1b** were all located from Δ*F* maps and refined freely.

The X-ray crystal structure of 2b

Reciprocal space analysis of the data set for the structure of **2b** clearly showed the crystal to be twinned. Unfortunately, despite numerous efforts no attempts at modelling the twinning gave any noticeable improvement over the standard, non-twin, data processing. The best that could be achieved was to process the data using every available crystal movement option (moderate and significant wobbling, as well as sudden discontinuous changes of sample orientation) despite no evidence that the crystal in any way moved independently of the goniometer. However, signs of the unresolved twinning are evident in the final Δ*F* map, with two residual electron density peaks significantly larger than the rest, at *ca*. 2.55 and 2.27 eÅ^{-3} (the next four are 0.97, 0.84, 0.84 and 0.72 eÅ^{-3}). These peaks both sit less than 1 Å away from the palladium centre and are almost diametrically opposite to each other, subtending an angle of *ca*. 178° at the palladium. Whilst this is a pattern often seen around highly absorbing atoms, the peaks are somewhat larger than typically seen around a second row metal atom.

Since there seems no sensible chemical explanation for these peaks, it is most likely that they are artefacts of the unresolved twinning.

Unsurprisingly, the two expected Pd–H–Mg bridging hydrogen atoms could not be reliably located from Δ*F* maps, and so the atom list for the asymmetric unit is 2H low, and that for the unit cell 4H low, compared to what is actually presumed to be present.

The X-ray crystal structure of 2a

The structure of **2a** was found to have crystallographic C_2 symmetry about an axis that passes through P1 and Pd1, and bisects the Mg1–Pd1–Mg1A angle. The (*t*Bu)$_3$P moiety was found to be disordered about this axis, and this was modelled by using one complete, 50% occupancy orientation for the three *tert*-butyl groups (the phosphorus atom was not treated as disordered), with the operation of the C_2 symmetry generating a second orientation of the same occupancy. The geometry of the unique orientation was optimised, the displacement parameters of adjacent, chemically-equivalent, atoms were restrained to be similar, and all of the non-hydrogen atoms were refined anisotropically. It is worth noting that a quick solution and refinement in the lower symmetry space group without the C_2 axis (*Ia*) retained the disorder in the phosphine, and so the model using the higher symmetry space group was preferred.

The included hexane solvent molecule was found to be disordered. Two orientations were identified of *ca*. 61 and 39% occupancy, their geometries were optimised, the displacement parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientation were refined isotropically). The unique Pd–H–Mg bridging hydrogen atom was located from a Δ*F* map and refined freely.

The X-ray crystal structure of 2c

The structure of **2c** was found to contain two crystallographically independent complexes, **2c-A** and **2c-B**, in the asymmetric unit. The C67-based cyclohexyl ring in molecule **2c-A**, and the C42-based *iso*-propyl group and C67-based cyclohexyl ring in molecule **2c-B**, were all found to be disordered, and in each case two orientations were identified, of *ca*. 54:46, 51:49 and 64:36% occupancy respectively. The geometries of each pair of orientations were optimised, the displacement parameters of adjacent atoms were restrained to be similar, and

only the non-hydrogen atoms of the major occupancy orientations were refined anisotropically (those of the minor occupancy orientations were refined isotropically).

The included solvent was found to be highly disordered, and the best approach to handling this diffuse electron density was found to be the SQUEEZE routine of PLATON.[15] This suggested a total of 271 electrons per unit cell, equivalent to 67.8 electrons per asymmetric unit. Before the use of SQUEEZE the solvent clearly resembled hexane (C_6H_{14}, 50 electrons) in multiple sites, and 1.35 hexane molecules corresponds to 67.5 electrons, so this was used as the solvent present. As a result, the atom list for the asymmetric unit is low by 2 x 1.35(C_6H_{14}) = $C_{16.2}H_{37.8}$ (and that for the unit cell low by $C_{32.4}H_{75.6}$) compared to what is actually presumed to be present.

The four Pt–H–Mg bridging hydrogen atoms (two in each independent molecule) were all located from Δ*F* maps and refined freely.

The X-ray crystal structure of 3

All three of the included benzene solvent molecules in the structure of **3** were found to be disordered, and two orientations of *ca*. 71:29, 73:27 and 65:35% occupancy were identified for the C111-, C121- and C131-based molecules respectively. The geometries of each pair of orientations were optimised, the displacement parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientations were refined anisotropically (those of the minor occupancy orientations were refined isotropically). The three Pd–H–Mg bridging hydrogen atoms were all located from Δ*F* maps and refined freely.

Table S3. Comparison of key bond angles around Pd in **1a** and **1b** from X-ray diffraction.

Angle	1a (º)	1b (º)
Mg1–Pd1–H1	67(2)	60(1)
Mg2–Pd1–H1	55(2)	58(1)
Mg2–Pd1–H2	65(2)	66(1)
Mg3–Pd1–H2	59(2)	56(1)
Mg3–Pd1–H3	54(2)	62(1)
Mg1–Pd1–H3	60(2)	58(1)

Figure S13**.** The structure of **1a** (X-ray diffraction: 50% probability ellipsoids).

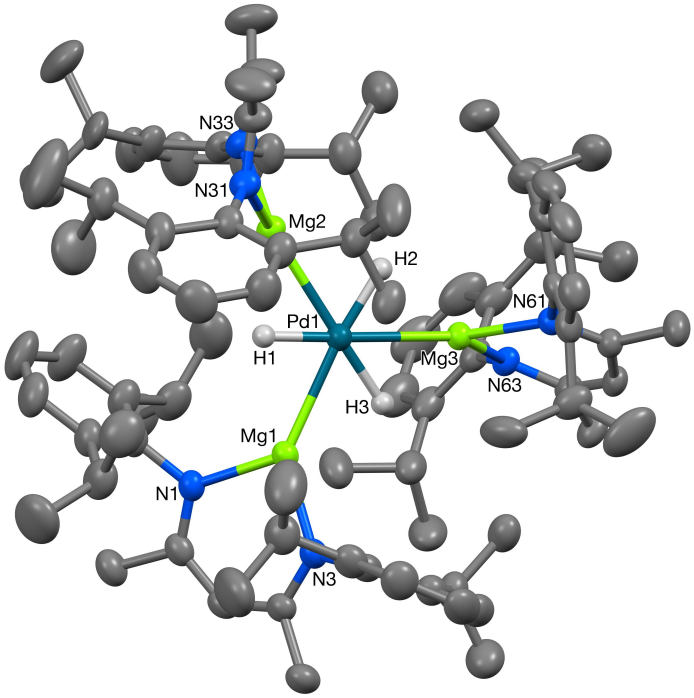


Figure S14. The structure of **1b** (X-ray diffraction: 50% probability ellipsoids).

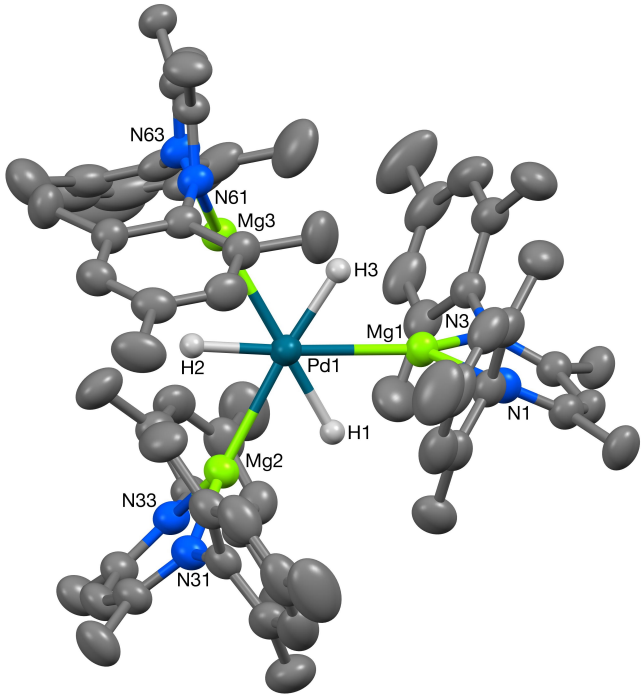


Figure S15. The structure of **2b** (X-ray diffraction: 50% probability ellipsoids).

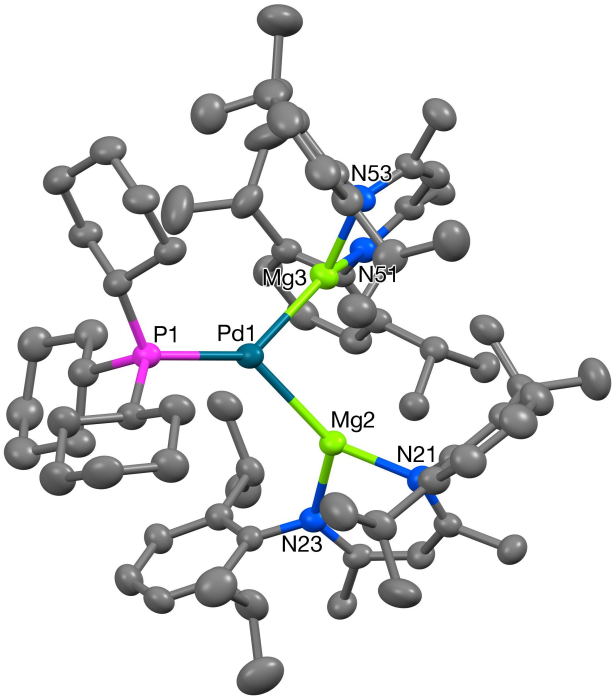


Figure S16. The structure of **2a** (X-ray diffraction: 50% probability ellipsoids).

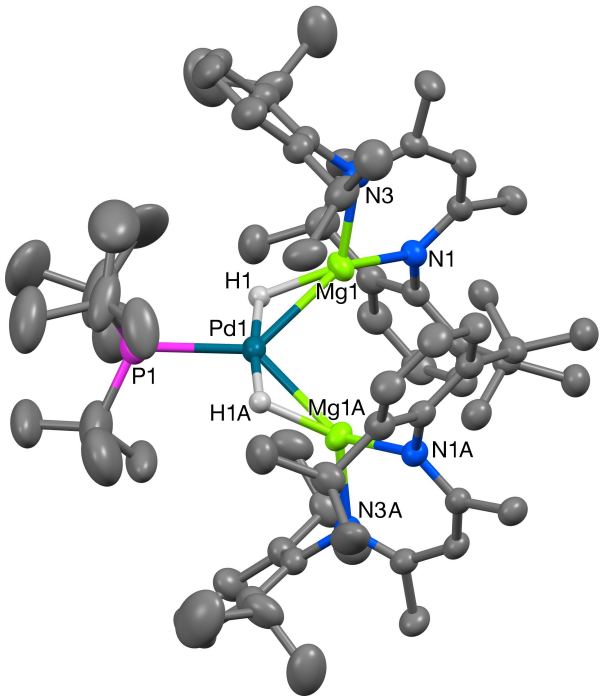


Figure S17**.** The structure of **2c-A**, one of the two independent complexes present in the crystal **2c** (X-ray diffraction: 50% probability ellipsoids).

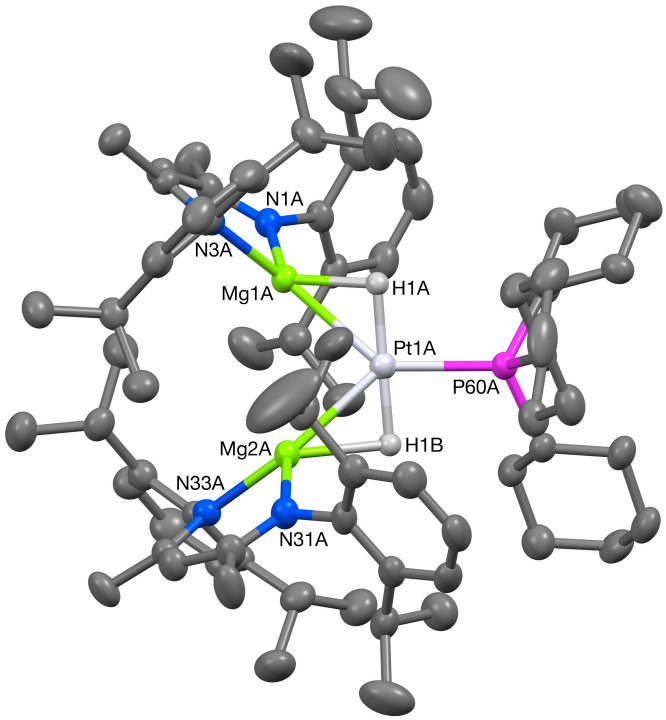
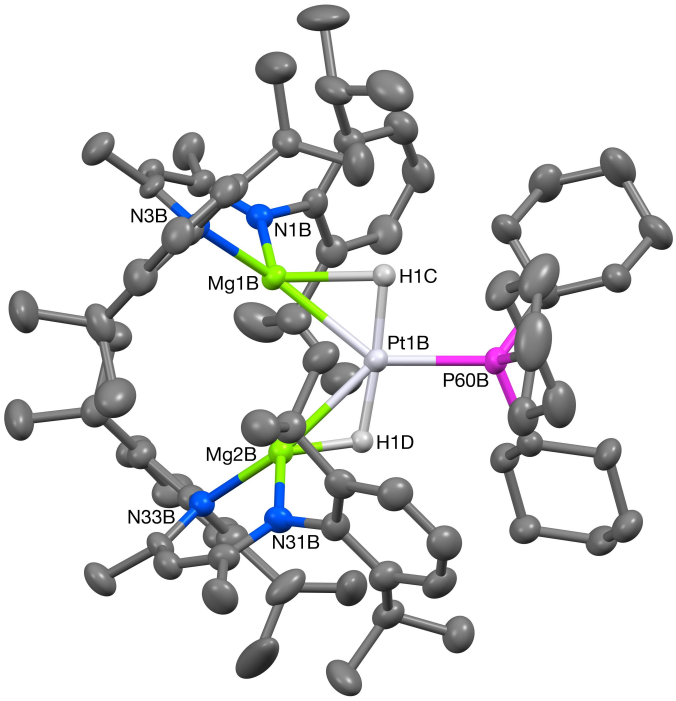


Figure S18**.** The structure of **2c-B**, one of the two independent complexes present in the crystal **2c** (X-ray diffraction: 50% probability ellipsoids).



The neutron diffraction structure of 3

The neutron diffraction data obtained for **3** has been modelled using the CRYSTALS software package.[16] Atoms of **3** are modelled using a composite approach to atomic sites and displacement parameters with all non-hydrogen atoms, the hydride hydrogens and the hydrogens not associated with methyl groups included with anisotropic displacement parameters and supported by a suitable set of restraints to augment the data.[17] All but three of the methyl groups are modelled with discrete hydrogen atom sites consistent with Fourier difference maps, and the remaining three methyl groups' hydrogen atoms are modelled using the "special shapes" facility[18] of CRYSTALS, again consistent with the observed residual nuclear density distribution. The included solvent (a mixture of benzene with some toluene) is likewise modelled using the same facility but in this case the model consists of, a combination of fractionally occupied isotropic atoms refined at the observed dominant sites of the disordered solvent rings combined with rings which represent the disordered aspects of the included solvent. No attempt to account for the fractionally occupied disordered methyl groups of toluene was made.

In the case of three methyl groups and the solvent molecules high occupancy (Occ>1) "atoms" appear in the model presented in the CIF (CCDC number 1946045). They describe the nuclear density modelled to best fit to the observed data using the advanced refinement method available in CRYSTALS which facilitates modelling of continuously disordered atomic scattering density as a "special shape" in this case a ring (for which there is no formal CIF description) which is applicable both to benzene rings and the disordered methyl hydrogens. The refinement software interprets the density as being distributed around the ring, not at the coordinate of the ring centre. This method was described by Schröder and co-workers[18] and has been found to be particularly applicable to the optimal refinement of structures from Laue neutron diffraction. At convergence R_1 = 0.1117, wR_2 = 0.0985 for I > 3σ(I). Max. and min. residual difference densities: 1.16 and –1.50 fermi A^{-3}.

Figure S19. One of the Laue images from which the single-crystal neutron diffraction data were extracted.

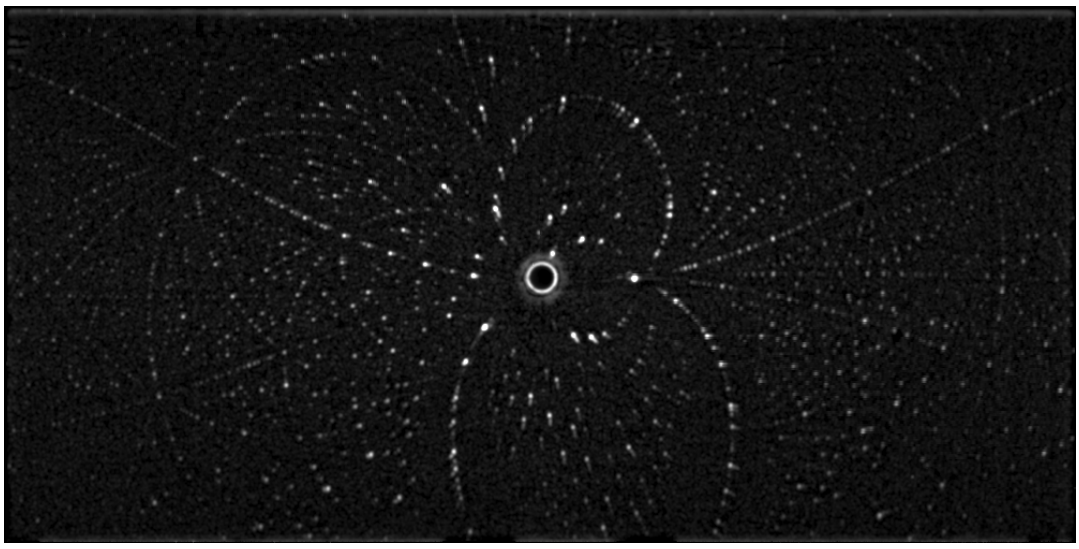


Figure S20. The molecular structure of **3** (a) X-ray diffraction: 50% probability ellipsoids, (b) neutron diffraction 50% probability ellipsoids, (c) displacement ellipsoid representation of metal coordination environment from neutron and (d) nuclear density for the hydrides shown with contours drawn at -1.0, -2.0 and -3.0 fermi $Å^{-3}$; selected atoms shown for clarity.

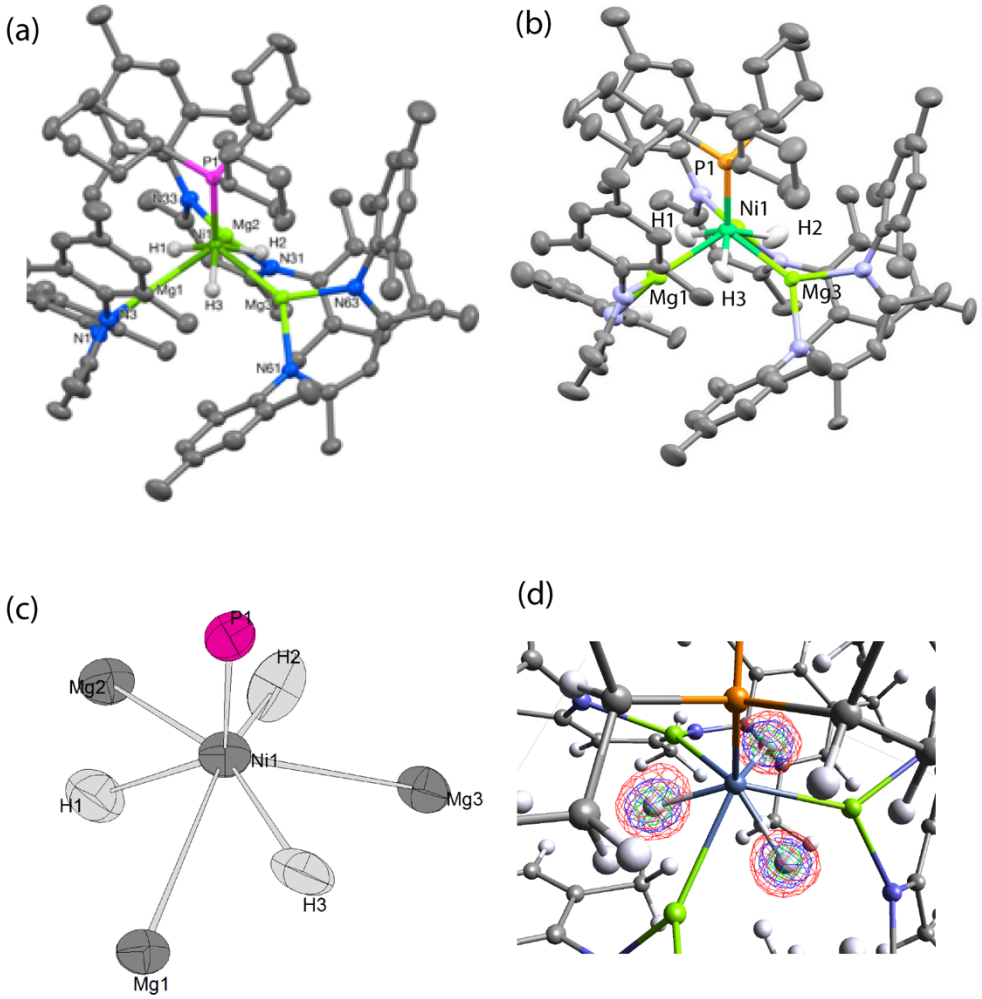


Table S4. Comparison of key bond lengths in **3** from X-ray and Neutron diffraction.

Bond length	X-ray (Å)	Neutron (Å)
Ni1–P1	2.1945(5)	2.217(17)
Ni1–Mg1	2.4548(7)	2.471(16)
Ni1–Mg2	2.4858(7)	2.480(16)
Ni1–Mg3	2.4861(7)	2.480(16)
Ni1–H1	1.53(3)	1.59(2)
Ni1–H2	1.50(2)	1.64(3)
Ni1–H3	1.55(2)	1.61(3)
Mg1–H1	2.01(2)	2.03(3)
Mg2–H2	2.05(2)	2.03(3)
Mg3–H3	1.98(2)	2.04(3)

5. DFT calculations

5.1 Methods

The geometries of products were optimised with the ωB97x hybrid exchange-correlation DFT functional using the Gaussian09 program package.[19] Stationary points were characterised depending on their imaginary frequencies (0 for minima and 1 for TSs). NBO analysis was performed using the NBO 6.0 version program.[20] QTAIM analysis was conducted with the AIMAll package.[21] Non-covalent interactions were analysed with the NCIPLOT 3.0 program.[22]

A benchmarking of the level of theory was performed by comparing computed structures with X-ray diffraction data. Some of the most widely employed DFT functionals were benchmarked,[23] and the ωB97x functional generally provided a very good agreement with the experimental geometries. This is consistent with previous benchmarking analysis done in the group.[24]

A combined basis set was employed. The SDD effective core potential was used for all metals (SDDAll). The split-valence 6-31G* basis set was used for C and H atoms. The basis set for metal hydrides was expanded by adding one extra set of diffuse functions and three sets of p- and one set of d- polarisation functions, *i.e.* formally [6-31++G(d,3pd)]. The triple-ξ 6-311+G* basis set was used for heteroatoms. This basis set provided very similar results to the 6-31+G(d,p) basis set, but it was much more efficient in terms of computational cost.

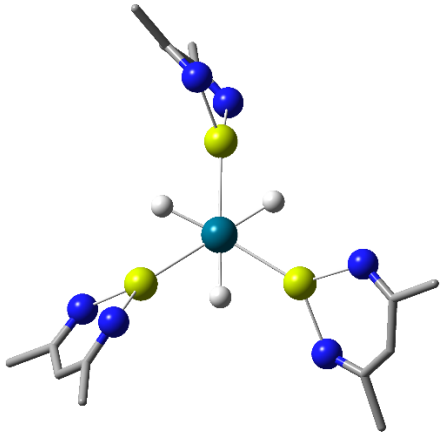
C H 0
6-31G*
****
N P 0
6-311+G*
****
75 201 0 *(atoms 75 and 201 are the hydrides)*
S 1 1.00
0.0360000 1.0000000
P 1 1.00
3.0000000 1.0000000
P 1 1.00
0.7500000 1.0000000
P 1 1.00
0.1875000 1.0000000
D 1 1.00
1.0000000 1.0000000
****
Pd Mg 0
SDDAll

The default numerical integration grid was also improved using a pruned grid with 99 radial shells and 590 angular points per shell (int=ultrafine). For the discussion of the computed

geometries, no significant difference was observed when optimising the structures using tight convergence criteria. Nevertheless, the reported coordinates (and further structural analysis) were obtained from the tightly optimised geometries (opt=tight).

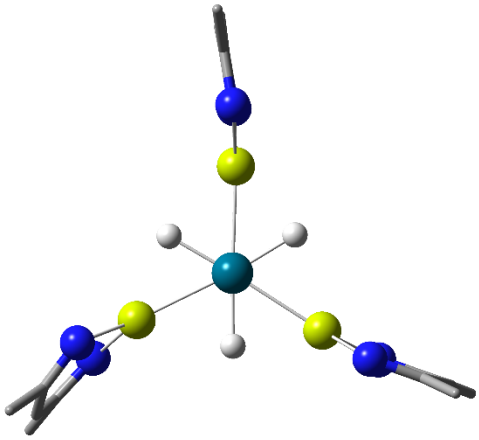
5.2 Calculated Geometries

Table S5. Comparison of selected computed and experimental bond lengths for compound **1a** (the ligands on Mg have been cut down for clarity).



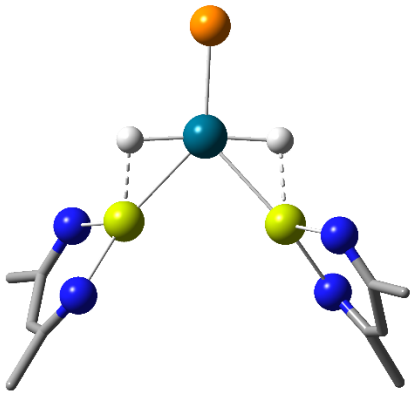
Bond	Calc.	Exp. (X-ray)
Pd–H	1.71, 1.72, 1.72	1.58, 1.58, 1.64
Pd–Mg	2.54, 2.55, 2.56	2.55, 2.56, 2.57
Mg–H	(2.16, 2.17), (2.26, 2.38), (2.15, 2.38)	(2.08, 2.23), (2.21, 2.39), (2.11, 2.43)

Table S6. Comparison of selected computed and experimental bond lengths for compound **1b** (the ligands on Mg have been cut down for clarity).



Bond	Calc.	Exp. (X-ray)
Pd–H	1.72, 1.73, 1.73	1.75, 1.72, 1.76
Pd–Mg	2.52, 2.52, 2.52	2.49, 2.50, 2.49
Mg–H	(2.35, 2.14), (2.34, 2.14), (2.28, 2.12)	(2.39, 2.10), (2.28, 2.14), (2.22, 2.15)

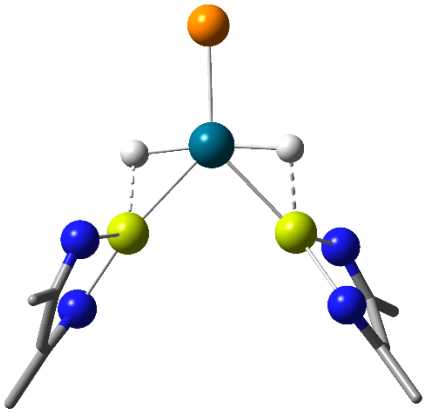
Table S7. Comparison of selected computed and experimental bond lengths for compound **2b** (the ligands have been cut down for clarity).



Bond	Calc.	Exp. (X-ray) [a]
Pd–H	1.67, 1.67	-
Pd–Mg	2.61, 2.62	2.61, 2.61
Mg–H	1.92, 1.90	-
Mg---Mg	3.60	3.64
Pd–P	2.46	2.40

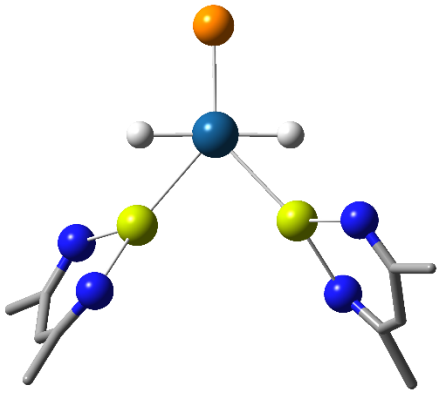
[a] The hydrides could not be located for this complex.

Table S8. Comparison of selected computed and experimental bond lengths for compound **2a** (the ligands have been cut down for clarity).



Bond	Calc.	Exp. (X-ray)
Pd–H	1.67, 1.68	1.59, 1.59
Pd–Mg	2.64, 2.62	2.60, 2.60
Mg–H	1.91, 1.87	1.80, 1.80
Mg---Mg	3.71	3.82
Pd–P	2.55	2.44

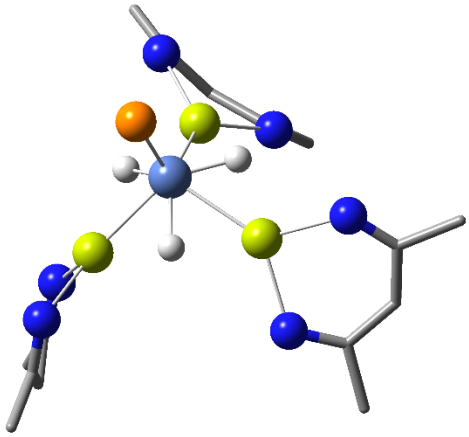
Table S9. Comparison of selected computed and experimental bond lengths for compound **2c** (the ligands have been cut down for clarity).



Bond	Calc.	Exp. (X-ray), polymorph 1 [a]	Exp. (X-ray), polymorph 2
Pt–H	1.66, 1.66	1.68, 1.60 (molec.1) 1.61, 1.53 (molec.2)	-
Pt–Mg	2.61, 2.62	2.59, 2.60 (molec.1) 2.58, 2.59 (molec.2)	2.59, 2.59
Mg–H	1.99, 2.00	1.65, 2.19 (molec.1) 1.88, 2.14 (molec.2)	-
Mg---Mg	3.51	3.46 (molec.1) 3.54 (molec.2)	3.47
Pt–P	2.40	2.35 (molec.1) 2.36 (molec.2)	2.34

[a] This complex has been crystallised as two different polymorphs. Polymorph 1 contained two molecules in the asymmetric unit. The hydrides could not be located from polymorph 2.

Table S10. Comparison of selected computed and experimental bond lengths for compound **3** (the ligands have been cut down for clarity).



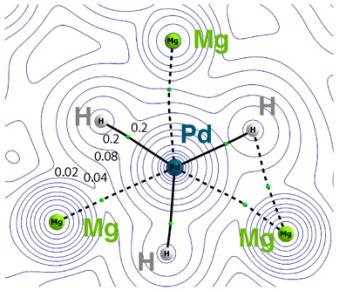
Bond	Calc.	Exp. (X-ray)	Exp. (Neutron)
Ni–H	1.60, 1.60, 1.61	1.50, 1.53, 1.56	1.59,1.61,1.64
Ni–Mg	2.45, 2.48, 2.48	2.46, 2.49, 2.49	2.47,2.48,2.48
Mg–H	(2.00, 2.02), (2.06, 2.07), (2.00, 2.05)	(2.01, 2.04), (2.01, 2.05), (1.98, 2.05)	2.03, 2.03, 2.04
Ni–P	2.24	2.19	2.22

For esd on the experimental data see table S4

5.3 QTAIM analysis and Non-Covalent Interactions (NCI) analysis

Figure S21. QTAIM molecular graph and associated data for the series **1a, 1b, 2b, 2a, 2c, 3**.

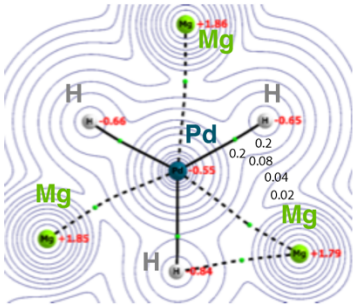
1a



*p*bcp
Pd–Mg 0.02
Pd–H 0.08–0.11
(Mg---H) 0.02

∇^2*p*bcp
Pd–Mg 0.11–0.13
Pd–H 0.26–0.44

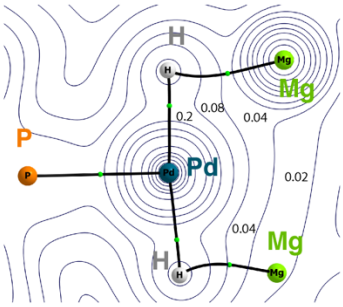
1b



*p*bcp
Pd–Mg 0.02
Pd–H 0.08–0.10
(Mg---H) 0.02

∇^2*p*bcp
Pd–Mg 0.12–0.13
Pd–H 0.27–0.42

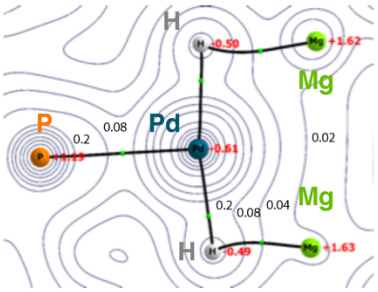
2b



*p*bcp
Pd–H 0.11
Mg–H 0.04

∇^2*p*bcp
Pd–H 0.17–0.18
Mg–H 0.13–0.14

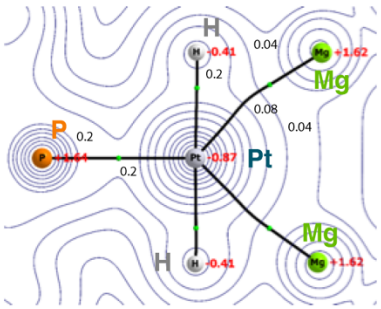
2a



*p*bcp
Pd–H 0.11
Mg–H 0.04

∇^2*p*bcp
Pd–H 0.18
Mg–H 0.14–0.15

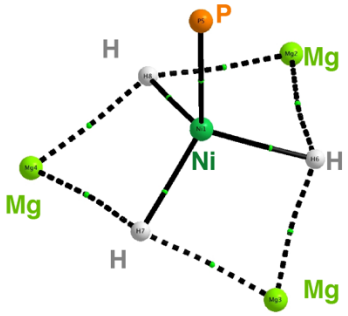
2c



*p*bcp
Pt–H 0.13
Mg–H 0.03

∇^2*p*bcp
Pt–H 0.14
Mg–H 0.11

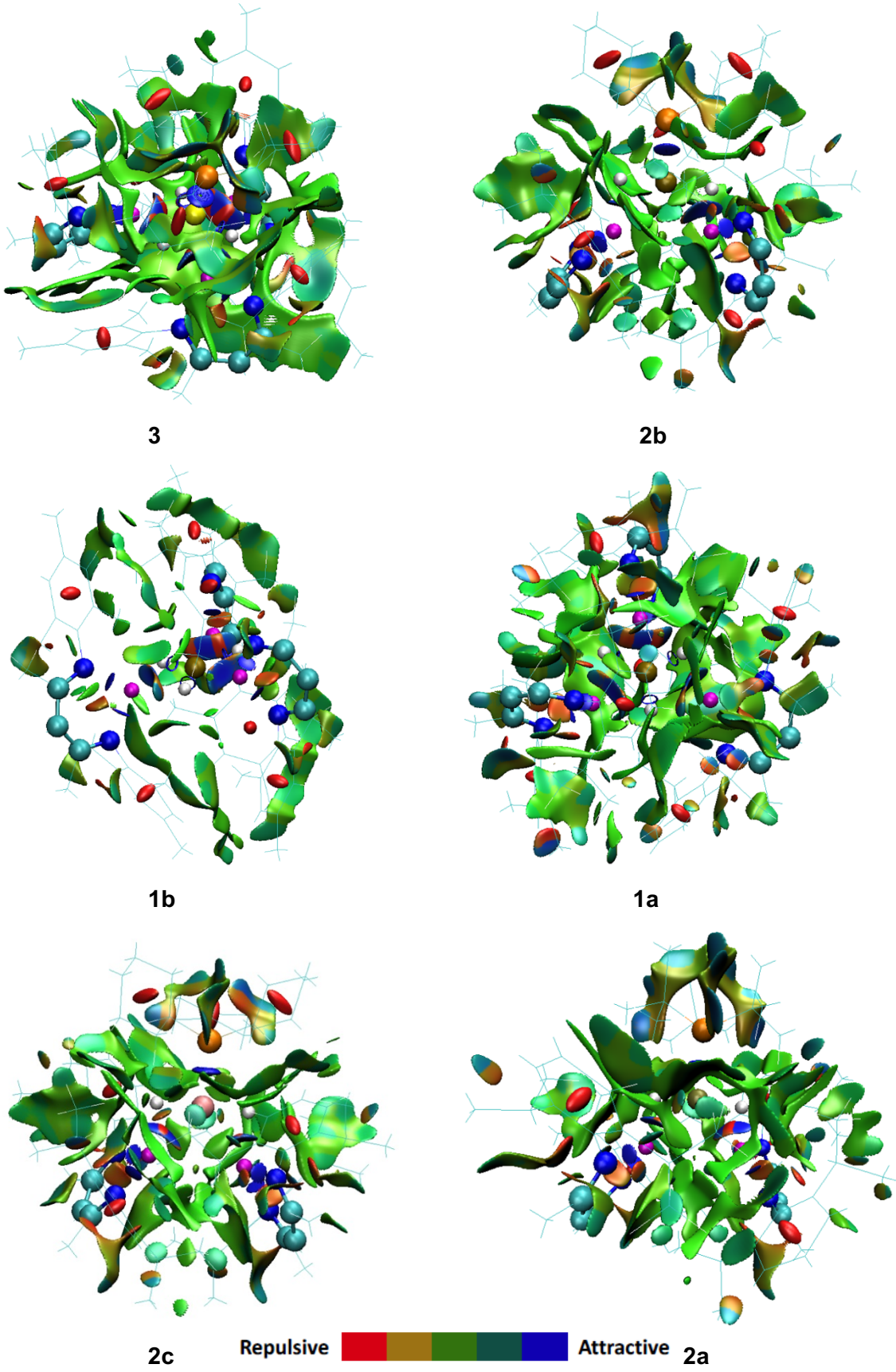
3



*p*bcp
Ni–H 0.08
Ni–P 0.07
Mg–H 0.02

∇^2*p*bcp
Ni–H 0.52-0.54
Ni–P 0.32
Mg–H 0.12–0.14

Figure S22. Non-covalent interaction (NCI) plots of complexes **1a**, **1b**, **2b**, **2a**, **2c** and **3**.



5.4 NBO analysis

Table S11. Selected Wiberg bond indexes (WBI).

Bond	2b	2a	2c	3	1a	1b
TM–H	0.38, 0.37	0.36, 0.37	0.43, 0.43	0.23, 0.21, 0.21	0.29, 0.28, 0.31	0.28, 0.29, 0.30
TM–Mg	0.23, 0.23	0.22, 0.21	0.26, 0.26	0.08, 0.07, 0.08	0.12, 0.12, 0.10	0.11, 0.12, 0.12
Mg–H	0.20, 0.20	0.20, 0.20	0.14, 0.14	0.10, 0.10, 0.10, 0.11, 0.10, 0.11	0.11, 0.09, 0.09, 0.13, 0.11, 0.10	0.09, 0.13, 0.13, 0.09, 0.13, 0.09
Mg---Mg	0.07	0.05	0.09	-	-	-
TM–P	0.16	0.14	0.23	0.32	-	-

Table S12. Selected NPA charges.

Atom	2b	2a	2c	3	1a	1b
Mg	1.51, 1.51	1.55, 1.56	1.50, 1.49	1.70, 1.70, 1.70	1.66, 1.66, 1.68	1.64, 1.65, 1.65
TM	-0.31	-0.30	-0.43	-0.29	-0.44	-0.42
H	-0.48, -0.48	-0.50, -0.50	-0.41, -0.41	-0.66, -0.67, -0.67	-0.61, -0.62, -0.60	-0.61, -0.61, -0.60
P	0.86	0.89	0.90	0.85	-	-

5.5 Potential Energy Surface Scans on $[Pd(H)_3(Mg)_3]^{3+}$ and $[Pd(H)_2(Mg)_2(PH_3)]^{2+}$

These complexes and in particular the hexagonal planar **1a** can be further inspected by generating simple models. The high ionic character of the Mg–N bonds to the diketiminate ligands mean that $[PdH_3Mg_3]^{3+}$ is a reasonable model for complexes **1a** and **1b**. $[PdH_3Mg_3]^{3+}$ can be freely optimised and the hexagonal planar geometry is as expected a minimum of the Potential Energy Surface (PES). This small model system allowed a more detailed analysis of the bonding configuration of the hexagonal planar arrangement.

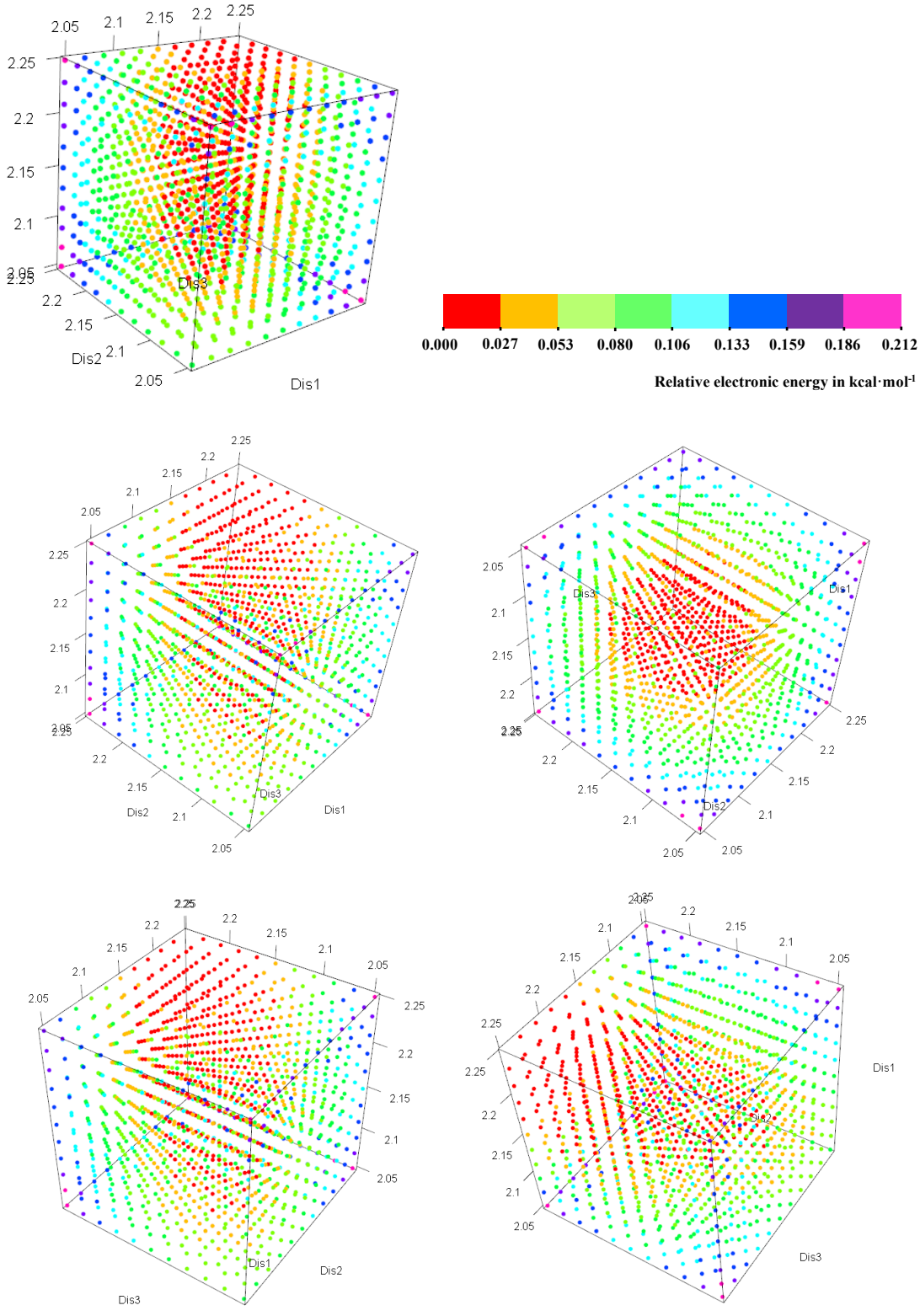
In order to explore the PES, an (relaxed) energy scan of the three Mg–H bonds was performed. We found that the energy cost of compressing the Mg–H bonds (from 2.25 Å to 2.05 Å) was very small, *i.e.* less than 0.3 kcal·mol^{-1}. In order to obtain data as reliable as possible, the scans were repeated using different levels of theory. Different DFT functionals (ωB97x, M06L

and B3PW91) provided similar trends[ii] and the effect of different basis sets was also small. Consequently, a bigger basis set (BS2) was employed for these models, in order to improve accuracy. BS2 consisted of the SDD effective core potential for Pd and the def2-QZVPP basis set for the rest of atoms.

The scan of the three Mg---H distances (performed at ωB97x/BS2) provided a clear picture of the PES, indicating that the ideal (almost D_{3h} symmetric) hexagonal planar geometry was the global minimum of the PES. This geometry, with all six Mg---H distance being 2.22 – 2.23 Å long, was independently optimised to confirm its nature as minimum and obtain further bonding analysis (*vide infra*). The PES can be graphically represented by plotting the three scanned Mg---H distances in the x,y,z axis, respectively. The energy corresponding to each point can be represented with a colour code, allowing this way to represent graphically the 4 variables.

[ii] The minimum found with DFT could also be found (with insignificant differences in the Mg–H distances) from a free optimisation of $[PdMg_3H_3]^{3+}$ using second-order Møller-Plesset perturbation theory (MP2).

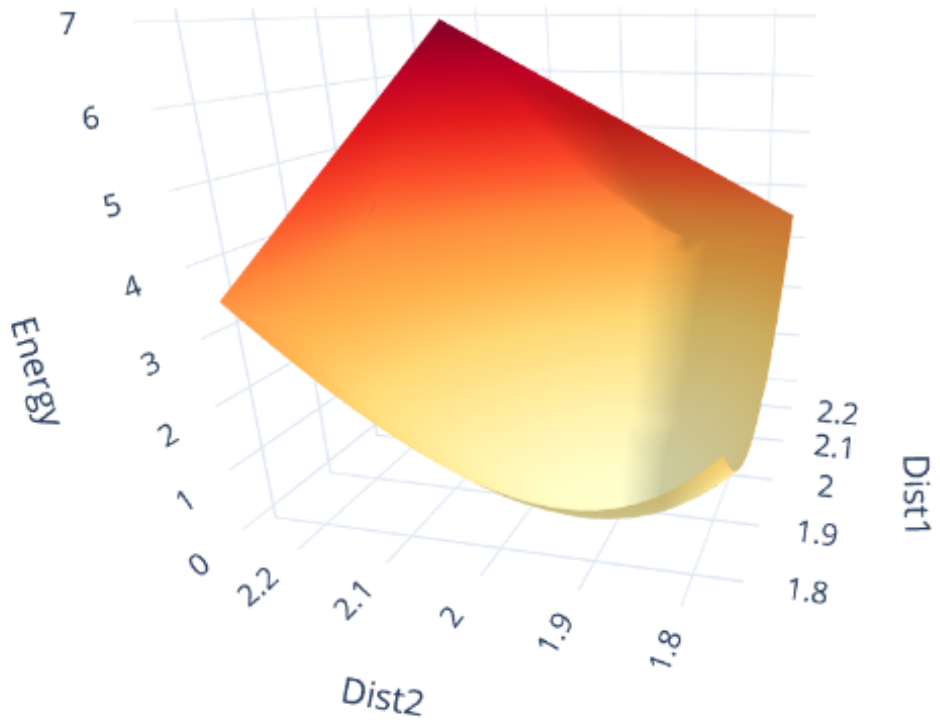
Figure S23. Different views of the PES obtained by plotting the three Mg---H distances (in Å) against electronic energy (kcal mol^{-1}).



This representation of the PES was constructed using a grid of 11x11x11 points (with a 0.02Å step) from Mg–H distances range from 2.25 Å to 2.05 Å. Careful inspection of the 1331 points of this grid allowed us to identify a single energy minimum corresponding to the (closest to) ideal hexagonal planar geometry, *i.e.* dist1=dist2=dist3=2.23 Å. The flat nature of the PES combined with the discrete nature of the grid make it impossible to confirm unambiguously the absence of other local minima, but this result strongly suggest that the hexagonal planar geometry is the only (and hence global) minimum of the PES. As can be inferred from Fig. S23, symmetric compression of the three Mg---H distances results in the lowest energetic path from the hexagonal planar geometry to the tris(σ-complex) type geometry.

A similar analysis of the PES can be done for complexes **2b** and **2a**, using another simple model, *i.e.* $[PdMg_2H_2(PH_3)]^{2+}$. The two Mg---H distances were scanned simultaneously in an analogous manner to that described above, using the same level of theory (ωB97x/BS2). In this case it was found that long Mg---H distances, came at a significant energetic cost.

Figure S24. PES of $[PdMg_2H_2(PH_3)]^{2+}$ obtained by plotting the two Mg–H distances (Å) against relative electronic energy (kcal·mol^{-1}).

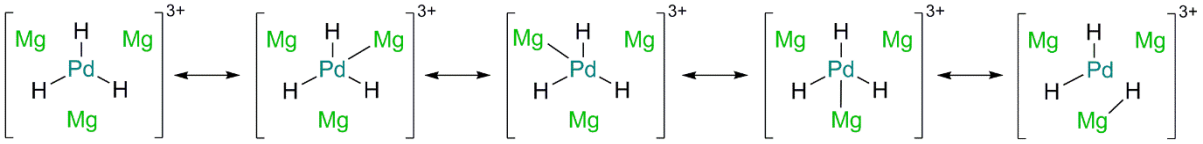


The PES was obtained by representing the two Mg---H distances (25x25 grid, step = 0.02 Å) against the electronic energy. As with the hexagonal planar model, a single minimum was found, but in this case, shorter Mg–H distances were significantly favoured. This geometry presents a T-shaped arrangement of the phosphine and the two hydride ligands around Pd, with a Mg–Pd–Mg angle near 90°. The minimum is found when the two Mg–H distances equal 1.91 Å, which is in perfect agreement with the calculated Mg–H distances in complexes **2b** and **2a** (*vide supra*). For this reason, they are best described as stretched bis(σ-complexes) and the geometry around Pd should be ascribed as trigonal planar.

5.6 NBO Analysis of $[Pd(H)_3(Mg)_3]^{3+}$

The bonding in the model, $[PdH_3Mg_3]^{3+}$, was further inspected by Natural Resonance Theory (NRT) analysis,[25] as implemented in the NBO 6.0 program. The main resonance forms identified by the NRT analysis are depicted in Figure S25.

Figure S25. Five main resonant forms identified by NRT analysis. The lone pairs on Pd (5 pairs on forms 1, 5 and 4 pairs on forms 2, 3, 4) have been omitted for clarity.



The Pd–Mg bonds were found to be essentially ionic in nature. The major contributing form is consistent with an electrostatic interaction between the Pd lone pairs and the cationic Mg centres. The following three equivalent resonant forms depict the small covalent contribution of the Pd–Mg bonds. The remaining resonant forms are minor contributors (less than 3% each). Some of these show the weak Mg–H interactions, as can be seen in the fifth resonant form in Fig. S25.

5.7 MO analysis of $[Pd(H)_3(Mg)_3]^{3+}$ and $[Pd(\eta^2\text{-}H_2)_3]$ and synthesised complexes

Figure S26. Qualitative MO diagram for $[Pd(H)_3(Mg)_3]^{3+}$ annotated with calculated MOs.

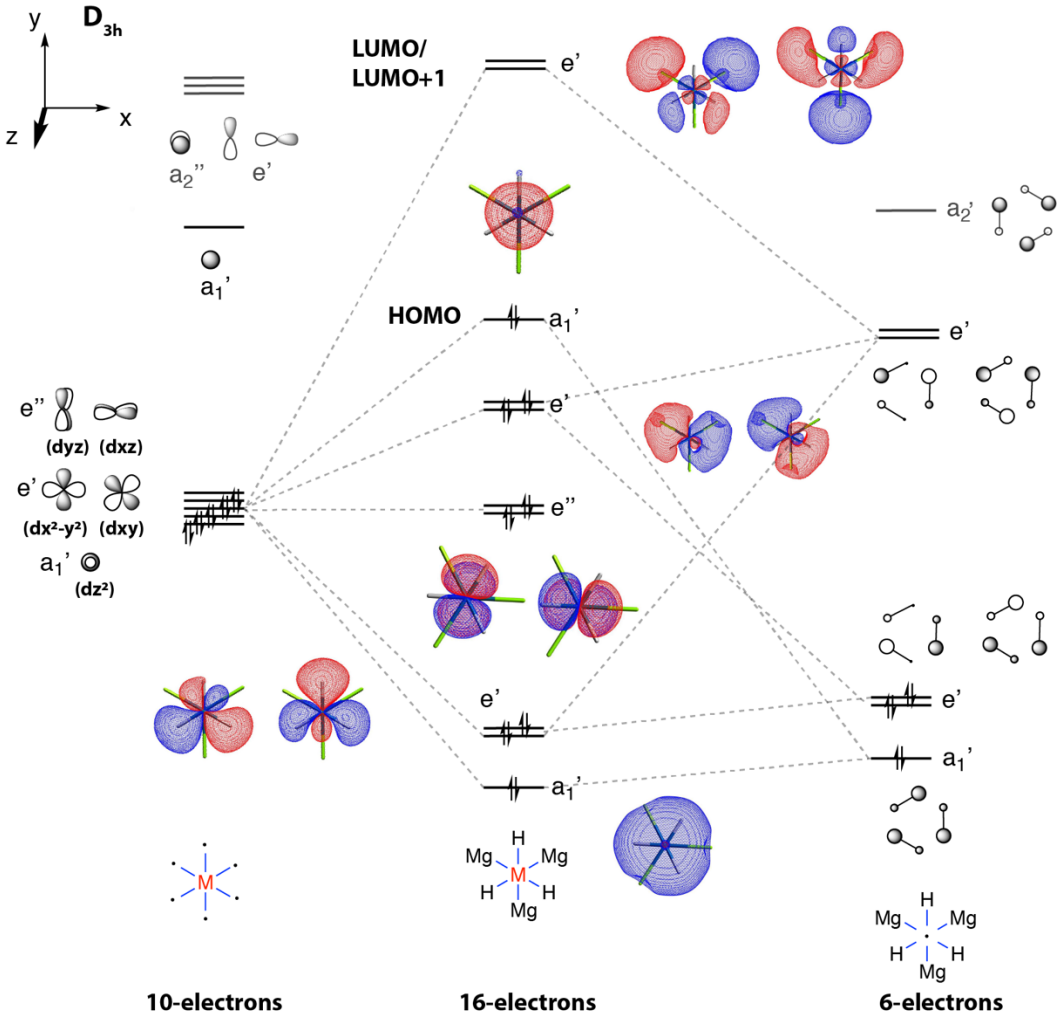


Figure S27. Qualitative MO diagram for [Pd(η^2-H_2)$_3$] annotated with calculated MOs.

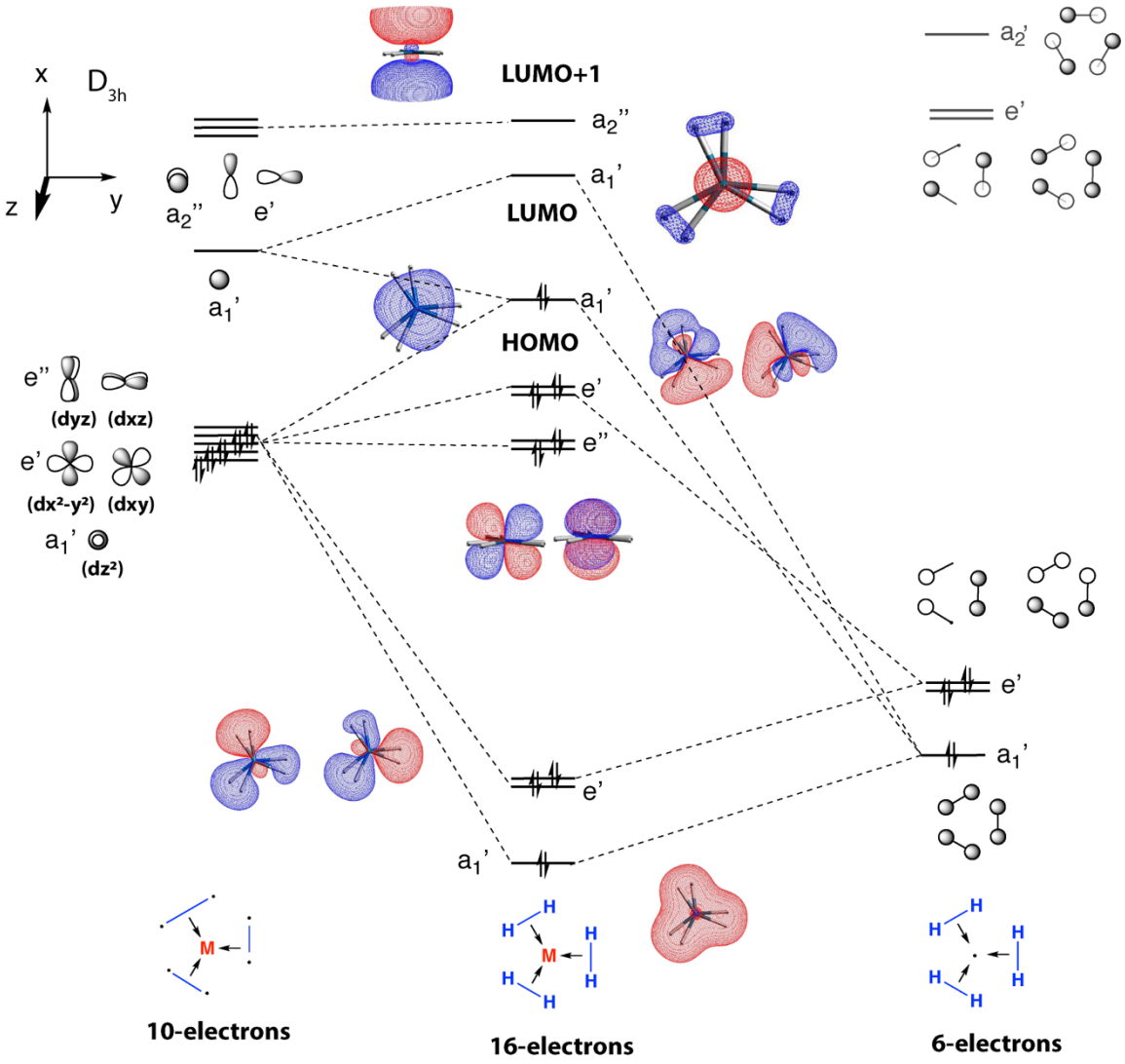


Figure S28. HOMO-LUMO gaps for complexes **1a**, **1b**, **2a**, **2b**, **2c** and **3**.

	HOMO (eV)	*LUMO (eV)*	*HOMO-LUMO gap (kcal/mol)*
1a	-0.27002	0.04869	7.35
1b	-0.27106	0.05496	7.52
2b	-0.24379	0.05347	6.85
2a	-0.24477	0.0524	6.85
2c	-0.246	0.05412	6.92
3	-0.2397	0.05793	6.86

6. XYZ coordinates

3

SCF (wB97x) = -4232.24681718
E(SCF)+ZPE(0 K)= -4230.307334
H(298 K)= -4230.196263
G(298 K)= -4230.457184
Lowest Frequency = 7.6548cm-1

Ni	-0.029992	-0.037702	0.207752
Mg	1.150579	-1.891326	-0.880000
Mg	-2.283042	0.043120	-0.827790
Mg	1.053951	1.993933	-0.702226
P	0.124925	-0.232285	2.437906
H	-0.774827	-1.311883	-0.431204
H	-0.815215	1.279685	-0.252174
H	1.446237	0.055790	-0.411735
N	0.720609	-3.180109	-2.476810
C	1.689370	-3.566926	-3.300046
C	3.063875	-3.402704	-3.047652
H	3.725123	-3.696059	-3.855865
C	3.698477	-3.132957	-1.817476
N	3.077332	-2.730459	-0.715520
C	1.340763	-4.278442	-4.594625
H	0.959575	-5.284690	-4.385365
H	2.220260	-4.373443	-5.235168
H	0.554412	-3.751490	-5.144031
C	5.195283	-3.379291	-1.785996
H	5.721211	-2.528575	-1.340414
H	5.584507	-3.545589	-2.793253
H	5.431142	-4.258278	-1.175192
C	-0.593964	-3.670029	-2.762167
C	-0.963142	-4.944987	-2.296756
C	-2.217957	-5.452215	-2.626699
H	-2.491494	-6.447112	-2.275025
C	-3.135018	-4.717105	-3.376724
C	-2.761372	-3.444461	-3.798155
H	-3.464747	-2.842039	-4.370994
C	-1.505320	-2.908066	-3.506796
C	-0.021046	-5.749848	-1.438076
H	0.135541	-5.252515	-0.471668
H	0.968976	-5.865396	-1.894439
H	-0.428452	-6.746318	-1.240022
C	-4.507863	-5.264346	-3.679588
H	-4.489085	-6.353301	-3.794533
H	-4.915447	-4.832219	-4.599513
H	-5.213034	-5.032954	-2.869730
C	-1.129736	-1.544461	-4.022675
H	-0.746793	-0.909276	-3.216298
H	-1.997029	-1.046510	-4.468210
H	-0.335421	-1.596099	-4.779321
C	3.818742	-2.806073	0.509445
C	4.482728	-1.686415	1.034616
C	5.155790	-1.809211	2.251142
H	5.681291	-0.938761	2.645438
C	5.193083	-3.006912	2.962780
C	4.550552	-4.111202	2.407673
H	4.579592	-5.065372	2.933577
C	3.865787	-4.032010	1.195041
C	4.500662	-0.376081	0.295903
H	3.551550	0.158914	0.420578
H	4.638106	-0.519201	-0.779257
H	5.309643	0.266297	0.661611
C	5.901800	-3.094488	4.291635
H	5.313198	-2.615805	5.084595
H	6.874020	-2.590432	4.259183
H	6.069554	-4.135347	4.586432
C	3.168881	-5.248234	0.640219
H	3.342027	-6.121321	1.277625
H	3.507060	-5.493219	-0.373766
H	2.086397	-5.083867	0.574003
N	-3.198818	1.213495	-2.340644
C	-4.054638	0.614482	-3.168123
C	-4.706746	-0.600510	-2.906114
H	-5.355396	-0.960335	-3.697436
C	-4.850454	-1.256725	-1.662677
N	-4.077531	-1.046788	-0.608129
C	-4.438470	1.287304	-4.474880
H	-5.116251	2.128972	-4.291898
H	-4.945035	0.581431	-5.137229
H	-3.561589	1.692520	-4.989204
C	-6.041084	-2.193170	-1.564837
H	-5.775708	-3.154850	-1.119327
H	-6.479099	-2.367386	-2.550107
H	-6.810297	-1.747286	-0.922435
C	-2.967105	2.605197	-2.595375
C	-3.921191	3.549874	-2.164969
C	-3.721356	4.898513	-2.444837
H	-4.468856	5.619062	-2.112186
C	-2.593806	5.351818	-3.130931
C	-1.663990	4.404796	-3.543129
H	-0.774528	4.727006	-4.080705
C	-1.831679	3.040235	-3.289190

C	-5.145176	3.123543	-1.395419
H	-5.837948	3.962622	-1.275794
H	-4.868545	2.770926	-0.395650
H	-5.682188	2.300923	-1.881349
C	-2.398065	6.821466	-3.411103
H	-3.244777	7.238201	-3.968854
H	-1.490870	6.994867	-3.999494
H	-2.307230	7.395856	-2.480996
C	-0.820840	2.055081	-3.809788
H	-1.231827	1.438201	-4.620275
H	-0.502937	1.357802	-3.027039
H	0.065241	2.573095	-4.189082
C	-4.505680	-1.622767	0.633342
C	-4.190057	-2.948332	0.973198
C	-4.680049	-3.467729	2.171032
H	-4.465616	-4.508088	2.414242
C	-5.423384	-2.702823	3.067670
C	-5.698257	-1.382255	2.722229
H	-6.281622	-0.760766	3.401371
C	-5.264778	-0.835559	1.513924
C	-3.364825	-3.815096	0.059154
H	-2.893083	-4.631929	0.617604
H	-2.579528	-3.241448	-0.443910
H	-3.972814	-4.271358	-0.731416
C	-5.903527	-3.294252	4.369802
H	-6.526304	-4.179986	4.198884
H	-6.495932	-2.572163	4.940625
H	-5.059406	-3.605436	4.996600
C	-5.618043	0.582661	1.152905
H	-6.165502	0.637122	0.204374
H	-4.714487	1.191418	1.028656
H	-6.232309	1.044423	1.932835
N	2.497075	2.457276	-2.170621
C	2.373983	3.589053	-2.863502
C	1.560712	4.674282	-2.496582
H	1.530216	5.495075	-3.205084
C	0.958021	4.933831	-1.246744
N	0.825275	4.039387	-0.279821
C	3.183361	3.784855	-4.133681
H	4.238679	3.962419	-3.897552
H	2.812839	4.642558	-4.699702
H	3.146999	2.894590	-4.769715
C	0.487897	6.358582	-1.024422
H	-0.529113	6.377321	-0.620488
H	0.507129	6.925829	-1.957970
H	1.131358	6.869256	-0.298709
C	3.616978	1.632490	-2.519238
C	4.896302	1.976445	-2.037456
C	5.997402	1.215254	-2.418654
H	6.983347	1.496949	-2.048563
C	5.871795	0.095996	-3.242392
C	4.597217	-0.243906	-3.682230
H	4.465372	-1.118838	-4.316999
C	3.467954	0.507486	-3.341044
C	5.082903	3.129418	-1.083897
H	4.677690	2.872609	-0.096135
H	4.569167	4.040387	-1.409619
H	6.145656	3.359057	-0.956352
C	7.080994	-0.721106	-3.625368
H	6.822019	-1.493355	-4.357186
H	7.516001	-1.222836	-2.752181
H	7.864603	-0.091962	-4.062811
C	2.123491	0.121005	-3.897314
H	1.760267	0.854103	-4.629546
H	1.366600	0.067595	-3.107635
H	2.174867	-0.857297	-4.385817
C	0.490549	4.518074	1.028748
C	-0.834495	4.519534	1.495317
C	-1.084071	4.942125	2.801157
H	-2.115118	4.963173	3.152800
C	-0.065635	5.352430	3.660557
C	1.234793	5.373368	3.163846
H	2.047842	5.712946	3.805196
C	1.527519	4.974899	1.859116
C	-1.976892	4.137843	0.592605
H	-2.112659	4.864087	-0.217859
H	-2.916526	4.084423	1.154937
H	-1.801327	3.170474	0.113449
C	-0.375174	5.759786	5.079879
H	-0.682136	4.894161	5.680109
H	-1.193895	6.487266	5.116593
H	0.497249	6.208527	5.565471
C	2.940965	5.048017	1.342129
H	3.035289	5.761242	0.513358
H	3.270186	4.079705	0.952499
H	3.631970	5.359392	2.132122
C	-0.017659	-1.961289	3.152502
H	-0.015258	-1.865791	4.245889
C	1.160031	-2.873059	2.783430
H	2.123926	-2.423722	3.047444
H	1.176103	-3.016220	1.690821
C	1.039513	-4.241901	3.459394
H	1.888808	-4.874226	3.173511
H	1.102907	-4.107022	4.550059
C	-0.283344	-4.923379	3.113555
H	-0.374495	-5.879760	3.644091

H	-0.298462	-5.157695	2.036597
C	-1.465586	-4.011192	3.440783
H	-1.518307	-3.864341	4.530957
H	-2.406364	-4.488671	3.145667
C	-1.330547	-2.647912	2.755395
H	-1.347244	-2.772686	1.664117
H	-2.198705	-2.023785	2.999755
C	-1.076561	0.738951	3.540641
H	-0.550278	1.690359	3.726143
C	-2.374565	1.099446	2.799174
H	-2.919649	0.176296	2.547775
H	-2.120808	1.590490	1.853002
C	-3.281556	2.008686	3.634535
H	-2.768178	2.967447	3.794757
H	-4.203682	2.231993	3.081611
C	-3.609773	1.392793	4.993578
H	-4.233544	2.074619	5.585594
H	-4.193518	0.471368	4.843980
C	-2.320598	1.056426	5.741323
H	-2.545643	0.586749	6.707459
H	-1.775016	1.987463	5.960969
C	-1.428564	0.127270	4.911475
H	-1.969198	-0.817989	4.763619
H	-0.528314	-0.115544	5.483855
C	1.793609	0.269275	3.161415
H	2.499527	-0.372506	2.613094
C	2.172593	1.719280	2.829767
H	1.484572	2.419356	3.326121
H	2.060474	1.895830	1.751357
C	3.610832	2.043763	3.249923
H	4.304412	1.437909	2.646944
H	3.834482	3.094829	3.030903
C	3.852293	1.755703	4.731856
H	4.901099	1.947127	4.991901
H	3.244861	2.445949	5.336559
C	3.465122	0.317977	5.074719
H	3.593313	0.132549	6.149047
H	4.133987	-0.378836	4.547528
C	2.017869	0.027590	4.664605
H	1.357329	0.690454	5.241988
H	1.762193	-1.001136	4.944155

2a

SCF (wB97x) = -3423.84875881
E(SCF)+ZPE(0 K)= -3422.155332
H(298 K)= -3422.061941
G(298 K)= -3422.280373

Lowest Frequency = 18.5617cm-1

Pd	0.010535	1.193880	0.072228
H	-1.430879	1.208729	-0.799131
Mg	-1.891318	-0.571833	-0.299369
P	0.201522	3.731052	0.138250
N	-2.580903	-2.044192	-1.610244
C	-3.541335	-2.903706	-1.285095
C	-4.207980	-2.933046	-0.045941
H	-4.897090	-3.759482	0.087997
C	-4.255079	-1.948745	0.959826
N	-3.518727	-0.844542	0.974662
C	-4.004536	-3.937671	-2.294590
H	-3.208465	-4.652475	-2.524331
H	-4.279959	-3.457706	-3.239450
H	-4.867380	-4.490305	-1.918442
C	-5.299374	-2.173766	2.036593
H	-4.908286	-1.925462	3.027286
H	-5.639891	-3.211557	2.035305
H	-6.169208	-1.528392	1.867260
C	-2.082279	-2.085157	-2.955727
C	-2.569451	-1.153046	-3.895279
C	-2.102103	-1.214103	-5.210035
H	-2.486790	-0.509416	-5.944577
C	-1.156200	-2.152712	-5.596798
H	-0.802365	-2.184939	-6.624418
C	-0.659452	-3.046018	-4.656285
H	0.089382	-3.775731	-4.958351
C	-1.110754	-3.036202	-3.335474
C	-3.606051	-0.097851	-3.532543
H	-3.783488	-0.154269	-2.452467
C	-3.103193	1.315836	-3.849552
H	-3.837675	2.064419	-3.528351
H	-2.939211	1.453118	-4.925314
H	-2.158500	1.521631	-3.333030
C	-4.947293	-0.375008	-4.223012
H	-5.336875	-1.364434	-3.956138
H	-4.847337	-0.336773	-5.314757
H	-5.693555	0.372997	-3.928599
C	-0.529224	-4.041474	-2.349932
H	-1.135858	-4.013856	-1.438463
C	-0.543359	-5.480616	-2.881700
H	-1.538035	-5.784340	-3.226504
H	-0.229514	-6.175720	-2.094137
H	0.149271	-5.606208	-3.722125
C	0.898212	-3.648275	-1.960870
H	0.921612	-2.635706	-1.538560
H	1.562882	-3.651970	-2.834441

H	1.317649	-4.337482	-1.219448
C	-3.935032	0.202198	1.865821
C	-3.287604	0.405935	3.098288
C	-3.733276	1.439241	3.927186
H	-3.244295	1.597056	4.886608
C	-4.784629	2.262575	3.555152
H	-5.117191	3.060233	4.215192
C	-5.407947	2.061831	2.329664
H	-6.229703	2.711974	2.036849
C	-5.006213	1.037332	1.473511
C	-2.140857	-0.471853	3.575865
H	-1.936517	-1.214606	2.797684
C	-2.516458	-1.233997	4.853411
H	-3.409497	-1.853790	4.707974
H	-2.722336	-0.544748	5.681653
H	-1.691834	-1.887868	5.158135
C	-0.857129	0.340625	3.786112
H	-0.552617	0.841085	2.858189
H	-0.038213	-0.318999	4.098303
H	-0.991380	1.104632	4.563813
C	-5.721760	0.858914	0.138333
H	-5.456514	-0.122966	-0.267539
C	-5.244776	1.909422	-0.870764
H	-4.160733	1.848468	-1.021061
H	-5.475313	2.923280	-0.519505
H	-5.735042	1.766266	-1.842610
C	-7.248798	0.896637	0.271861
H	-7.607430	0.181043	1.020786
H	-7.716455	0.646946	-0.687558
H	-7.609533	1.890533	0.561557
C	0.589650	4.455930	-1.593012
C	0.344111	5.961369	-1.786739
H	0.901035	6.580205	-1.078828
H	0.672067	6.242099	-2.797149
H	-0.714138	6.225838	-1.709642
C	-0.243149	3.694750	-2.643834
H	-1.313082	3.897967	-2.581430
H	0.090940	4.003324	-3.644148
H	-0.099748	2.615130	-2.554178
C	2.059402	4.159845	-1.941593
H	2.759696	4.800702	-1.398613
H	2.327297	3.112334	-1.760694
H	2.212186	4.353324	-3.011420
C	1.548845	4.376980	1.346518
C	1.925653	5.864330	1.231461
H	2.451900	6.080211	0.296733
H	1.069543	6.538395	1.304769
H	2.613903	6.115837	2.050063
C	2.844451	3.563958	1.166280
H	3.304705	3.685632	0.184939
H	3.568947	3.907974	1.917591
H	2.672069	2.496730	1.323526
C	1.101702	4.094173	2.793589
H	0.788612	3.051231	2.923045
H	1.956746	4.266254	3.460651
H	0.293475	4.747661	3.130873
C	-1.463792	4.483165	0.714619
C	-1.444624	5.943138	1.196302
H	-0.871936	6.076243	2.118016
H	-1.049112	6.632666	0.444537
H	-2.476347	6.251092	1.414087
C	-2.013860	3.596017	1.847045
H	-1.375281	3.559975	2.731300
H	-2.990033	3.986078	2.161672
H	-2.165951	2.567897	1.502063
C	-2.504116	4.382461	-0.415024
H	-2.526508	3.380779	-0.854317
H	-3.496054	4.577657	0.013744
H	-2.345062	5.116412	-1.209734
H	1.386416	0.917134	0.975122
Mg	1.769441	-0.767344	0.253026
N	2.362150	-2.436156	1.354862
C	3.248169	-3.316046	0.903108
C	3.909339	-3.218395	-0.336035
H	4.515463	-4.075619	-0.606287
C	4.051428	-2.094729	-1.173332
N	3.431157	-0.933972	-0.991636
C	3.631245	-4.509955	1.756660
H	2.770314	-5.157990	1.947634
H	3.999365	-4.177804	2.733416
H	4.411377	-5.101181	1.273628
C	5.037149	-2.253236	-2.315715
H	4.523207	-2.146344	-3.277166
H	5.517961	-3.233107	-2.286688
H	5.810750	-1.480020	-2.281374
C	1.898556	-2.582815	2.704894
C	2.504290	-1.808906	3.716932
C	2.052955	-1.944232	5.031088
H	2.522078	-1.357123	5.818430
C	1.018359	-2.812223	5.349901
H	0.677222	-2.906103	6.378055
C	0.419977	-3.559689	4.343404
H	-0.393095	-4.237295	4.596504
C	0.844848	-3.467484	3.017088
C	3.643647	-0.842788	3.422805
H	3.833399	-0.870347	2.344952

C	3.272565	0.597714	3.798295
H	4.068358	1.290608	3.495024
H	3.131962	0.704260	4.881272
H	2.344475	0.909661	3.305042
C	4.943800	-1.271502	4.113553
H	5.244726	-2.280497	3.808358
H	4.837385	-1.268089	5.205297
H	5.757881	-0.582975	3.854821
C	0.159068	-4.321625	1.957907
H	0.763667	-4.278762	1.045685
C	0.038058	-5.794462	2.370431
H	1.000535	-6.214637	2.683626
H	-0.337269	-6.390836	1.530640
H	-0.664807	-5.924157	3.201627
C	-1.223270	-3.761253	1.612175
H	-1.142843	-2.736910	1.228682
H	-1.873864	-3.728956	2.495901
H	-1.722811	-4.369548	0.849241
C	3.909107	0.192716	-1.743666
C	3.430199	0.447069	-3.042703
C	3.940156	1.542562	-3.743988
H	3.576285	1.748517	-4.748431
C	4.899894	2.370808	-3.183779
H	5.291822	3.215054	-3.745938
C	5.350100	2.124248	-1.891692
H	6.091634	2.788497	-1.457094
C	4.867351	1.047264	-1.146593
C	2.352839	-0.412382	-3.688065
H	2.246876	-1.325499	-3.093174
C	2.695723	-0.834818	-5.121503
H	3.676030	-1.322171	-5.184907
H	2.707056	0.022745	-5.804724
H	1.937198	-1.535149	-5.491085
C	1.004822	0.315470	-3.655162
H	0.714655	0.562974	-2.625987
H	0.215227	-0.306916	-4.090734
H	1.057506	1.252446	-4.226087
C	5.373251	0.806998	0.275889
H	4.499338	0.525500	0.878925
C	5.996546	2.047749	0.924528
H	5.363623	2.933494	0.825950
H	6.977507	2.277273	0.489784
H	6.154613	1.860893	1.993573
C	6.391194	-0.340997	0.368489
H	5.958823	-1.313181	0.121773
H	6.783406	-0.409436	1.391164
H	7.239885	-0.154209	-0.302121

2b

SCF (wB97x) = -3656.10617132
E(SCF)+ZPE(0 K)= -3654.297067
H(298 K)= -3654.201789
G(298 K)= -3654.427006
Lowest Frequency = 14.1727cm-1

Mg	-1.656125	1.312167	0.233096
N	-3.364592	1.387420	1.428651
C	-4.494818	1.965482	1.030180
C	-4.681118	2.600733	-0.211159
H	-5.691313	2.941281	-0.409303
C	-5.698377	1.986349	1.954296
H	-6.069825	0.974343	2.142007
H	-6.508877	2.578413	1.525451
H	-5.431609	2.410158	2.928076
C	-3.312645	0.905627	2.779658
C	-3.843369	-0.357385	3.119989
C	-3.796291	-0.769076	4.453218
H	-4.204693	-1.740589	4.725249
C	-3.253961	0.041354	5.442102
H	-3.243076	-0.289397	6.477783
C	-2.713473	1.270839	5.092745
H	-2.273571	1.899371	5.864470
C	-2.713660	1.714170	3.768501
C	-4.453098	-1.292403	2.083074
H	-4.559004	-0.735339	1.146080
C	-3.520579	-2.477375	1.812346
H	-2.538732	-2.133478	1.464908
H	-3.934865	-3.148890	1.051488
H	-3.353344	-3.066580	2.723298
C	-5.840838	-1.810553	2.483701
H	-5.784741	-2.484453	3.346659
H	-6.283781	-2.376948	1.655819
H	-6.527722	-0.998011	2.744684
C	-2.074393	3.058686	3.444673
H	-2.085619	3.188087	2.356305
C	-2.877928	4.220330	4.041828
H	-3.911036	4.219932	3.674906
H	-2.423854	5.181726	3.771697
H	-2.909948	4.160355	5.136745
C	-0.610560	3.103599	3.901499
H	-0.524583	3.004091	4.990318
H	-0.149706	4.056913	3.617606
H	-0.030718	2.295570	3.439533
N	-2.422944	2.731262	-1.073551
C	-3.713723	3.025023	-1.143415

C	-4.222521	3.943293	-2.237776
H	-3.792822	3.679010	-3.208291
H	-3.930786	4.979844	-2.033621
H	-5.311897	3.901792	-2.304502
C	-1.530305	3.502333	-1.890180
C	-1.141893	4.785045	-1.441995
C	-0.296847	5.548745	-2.244938
H	0.005099	6.540157	-1.912668
C	0.173075	5.065706	-3.460407
H	0.823700	5.679338	-4.079290
C	-0.188213	3.792495	-3.873275
H	0.186903	3.410615	-4.820856
C	-1.037298	2.991461	-3.104065
C	-1.595086	5.340642	-0.096338
H	-2.382266	4.688671	0.297066
C	-0.436764	5.316673	0.909756
H	-0.017291	4.307544	1.011159
H	-0.776761	5.651236	1.898510
H	0.371516	5.987021	0.590269
C	-2.182782	6.752778	-0.202166
H	-1.427359	7.485390	-0.510078
H	-2.573307	7.073249	0.770848
H	-3.003728	6.796622	-0.926987
C	-1.406832	1.609473	-3.618404
H	-2.062086	1.136666	-2.878704
C	-2.183502	1.683806	-4.939053
H	-3.098128	2.280423	-4.838024
H	-2.467108	0.676849	-5.265710
H	-1.576708	2.137381	-5.732623
C	-0.163055	0.725402	-3.765921
H	0.530886	1.133541	-4.513285
H	-0.451613	-0.282785	-4.085875
H	0.371286	0.641706	-2.811031
Pd	0.744025	0.312067	-0.026560
H	0.160655	1.692117	0.718931
P	3.087681	1.040709	0.070115
C	4.214309	0.257007	-1.206935
C	3.501488	0.060358	-2.559763
C	5.602071	0.879221	-1.447930
H	4.369639	-0.751079	-0.784889
C	4.345012	-0.779472	-3.524746
H	3.295824	1.040869	-3.015110
H	2.529179	-0.417373	-2.399197
C	6.444519	0.012986	-2.390342
H	5.479357	1.870613	-1.905880
H	6.140916	1.031528	-0.508529
C	5.740565	-0.190756	-3.731528
H	3.823653	-0.874388	-4.485904
H	4.441743	-1.798620	-3.119194
H	7.428356	0.475581	-2.539102
H	6.623168	-0.965667	-1.919213
H	6.337481	-0.839168	-4.384882
H	5.653755	0.779847	-4.242461
C	3.753901	0.428000	1.709735
C	5.277479	0.282065	1.878237
C	3.130651	1.232506	2.867255
H	3.330239	-0.588522	1.770455
C	5.644102	-0.267955	3.260952
H	5.777077	1.249294	1.740616
H	5.675253	-0.391849	1.109568
C	3.528433	0.668383	4.233391
H	3.453966	2.281969	2.816289
H	2.038448	1.236098	2.763252
C	5.047524	0.582208	4.382810
H	6.736077	-0.321947	3.356695
H	5.263880	-1.295215	3.348701
H	3.094307	1.287562	5.029282
H	3.103734	-0.338927	4.342143
H	5.312881	0.163048	5.361488
H	5.478908	1.594243	4.344866
C	3.342097	2.894650	0.051970
C	4.682143	3.477774	0.538643
C	2.958531	3.475770	-1.323125
H	2.566359	3.231808	0.758906
C	4.657322	5.009544	0.546562
H	5.501407	3.145026	-0.109359
H	4.913314	3.119640	1.546522
C	2.983967	5.007448	-1.322725
H	3.663398	3.115031	-2.086436
H	1.960787	3.122007	-1.617756
C	4.322379	5.561552	-0.837541
H	5.625434	5.392650	0.893083
H	3.902270	5.357442	1.267776
H	2.754721	5.376314	-2.329273
H	2.181977	5.375564	-0.667396
H	4.297362	6.658348	-0.819306
H	5.116921	5.275008	-1.543235
Mg	-0.419374	-2.027587	-0.258569
N	0.040525	-3.606544	1.007686
N	-1.616263	-3.248650	-1.450197
C	-0.682682	-4.715308	1.075703
C	1.226130	-3.539693	1.812255
C	-2.057202	-4.436205	-1.044017
C	-1.922969	-2.851037	-2.794072
C	-1.712366	-5.050984	0.174358
C	-0.385383	-5.743160	2.150120

C	2.438804	-4.014167	1.269908
C	1.186982	-3.001149	3.113127
C	-2.989196	-5.241557	-1.931222
C	-3.170680	-2.282641	-3.120825
C	-0.934822	-3.029118	-3.788793
H	-2.214078	-5.990683	0.375640
H	0.630259	-6.137920	2.039582
H	-1.090123	-6.575801	2.104777
H	-0.439056	-5.288083	3.144875
C	3.590017	-3.972575	2.058872
C	2.527903	-4.586389	-0.139449
C	2.359669	-2.992740	3.870112
C	-0.083633	-2.401822	3.693719
H	-3.971103	-4.761892	-1.997749
H	-3.126751	-6.250084	-1.536675
H	-2.599619	-5.313149	-2.951384
C	-3.427152	-1.948395	-4.452663
C	-4.242123	-2.002347	-2.075146
C	-1.247445	-2.702334	-5.108889
C	0.446871	-3.576073	-3.444517
H	4.528599	-4.346928	1.653871
C	3.554086	-3.482229	3.357596
H	1.524215	-4.566032	-0.577783
C	3.436234	-3.728054	-1.028268
C	2.994062	-6.047604	-0.134411
H	2.335099	-2.598708	4.884350
H	-0.909762	-2.654153	3.021307
C	-0.435390	-2.955820	5.078863
C	0.025643	-0.872809	3.738211
H	-4.387638	-1.510374	-4.716829
C	-2.486490	-2.172853	-5.446878
H	-3.943657	-2.494798	-1.143300
C	-4.336987	-0.499467	-1.792023
C	-5.622661	-2.541607	-2.473183
H	-0.505637	-2.850325	-5.888769
H	0.689123	-3.243999	-2.427038
C	0.470628	-5.110212	-3.435439
C	1.548599	-3.031482	-4.358388
H	4.453691	-3.482122	3.968836
H	3.052811	-2.703270	-1.104145
H	3.494516	-4.150154	-2.040011
H	4.457860	-3.680925	-0.629163
H	4.014176	-6.143322	0.256945
H	2.988859	-6.453628	-1.153256
H	2.339646	-6.675287	0.481215
H	-0.514999	-4.049563	5.074912
H	-1.395958	-2.542577	5.409260
H	0.315495	-2.679264	5.828819
H	0.817459	-0.559080	4.431941
H	-0.916039	-0.429358	4.077813
H	0.261113	-0.463647	2.746801
H	-2.710964	-1.922554	-6.480927
H	-3.385994	-0.108992	-1.410550
H	-5.113428	-0.280212	-1.050054
H	-4.575965	0.062821	-2.704003
H	-6.042122	-1.986136	-3.320190
H	-6.323136	-2.436451	-1.636211
H	-5.588111	-3.598998	-2.757954
H	-0.213335	-5.523435	-2.686544
H	1.479245	-5.475379	-3.202256
H	0.186363	-5.507014	-4.418323
H	1.480328	-3.439557	-5.374120
H	2.531801	-3.310777	-3.963960
H	1.509682	-1.937623	-4.423103
H	1.171811	-1.123604	-0.758915

1b

SCF (wB97x) = -3142.19669867
E(SCF)+ZPE(0 K)= -3140.756599
H(298 K)= -3140.664584
G(298 K)= -3140.887431
Lowest Frequency = 10.2628cm-1

Pd	-0.024161	-0.131822	-0.006804
Mg	0.344763	-2.526793	-0.682347
Mg	-0.333185	0.491841	2.412672
Mg	-0.061030	1.717364	-1.715363
H	-0.003614	-1.287539	1.276062
H	-0.265934	1.534189	0.386551
H	0.193528	-0.621972	-1.642810
N	1.968561	-3.766538	-0.828183
C	1.869321	-5.089679	-0.907639
C	0.660492	-5.800116	-1.029096
H	0.757358	-6.878975	-1.070653
C	-0.650990	-5.305828	-1.170417
N	-0.979869	-4.021914	-1.123031
C	3.132008	-5.929221	-0.874429
H	3.778312	-5.694994	-1.727225
H	2.896581	-6.994934	-0.898360
H	3.714643	-5.716603	0.028410
C	-1.735455	-6.340310	-1.398412
H	-2.519704	-6.254398	-0.638623
H	-1.327454	-7.352554	-1.370915
H	-2.219861	-6.184508	-2.368645
C	3.278820	-3.192153	-0.800838

C	3.932022	-2.902340	-2.009832
C	5.216931	-2.364401	-1.967970
H	5.734613	-2.164476	-2.906826
C	5.860650	-2.088018	-0.761769
C	5.176738	-2.353183	0.422232
H	5.656948	-2.140059	1.376685
C	3.892094	-2.898982	0.425451
C	3.256592	-3.179958	-3.329535
H	3.012828	-4.242245	-3.452214
H	3.896794	-2.880494	-4.165505
H	2.310516	-2.629682	-3.413675
C	7.255616	-1.512765	-0.749343
H	7.738201	-1.657286	0.222805
H	7.244400	-0.433545	-0.952774
H	7.886050	-1.979942	-1.513873
C	3.181870	-3.185089	1.724135
H	2.319142	-2.518275	1.854150
H	3.851754	-3.028261	2.574952
H	2.805685	-4.214162	1.765495
C	-2.343827	-3.656707	-1.348759
C	-3.215396	-3.504323	-0.260527
C	-4.535570	-3.124811	-0.504903
H	-5.211036	-3.005840	0.341551
C	-5.007961	-2.897284	-1.795590
C	-4.118499	-3.049000	-2.858640
H	-4.466953	-2.870954	-3.876171
C	-2.787023	-3.408142	-2.657347
C	-2.734006	-3.754942	1.146103
H	-2.255841	-4.736860	1.244785
H	-3.565525	-3.701914	1.854909
H	-1.993477	-3.002141	1.446660
C	-6.431622	-2.459963	-2.037033
H	-6.505056	-1.364602	-2.084902
H	-7.095042	-2.797263	-1.233556
H	-6.816976	-2.852659	-2.984087
C	-1.835409	-3.521589	-3.822007
H	-1.005813	-2.809623	-3.721508
H	-2.348477	-3.310316	-4.765398
H	-1.386714	-4.519685	-3.894014
C	0.633973	1.686883	4.981246
N	0.988489	1.144980	3.824117
C	-0.694853	1.799628	5.434670
H	-0.819393	2.278247	6.399395
C	-1.880864	1.344364	4.826784
N	-1.942019	0.744021	3.644231
C	1.708517	2.230581	5.901706
H	2.398015	1.435746	6.206220
H	1.272979	2.677415	6.797606
H	2.309888	2.987409	5.386253
C	-3.162399	1.575247	5.603099
H	-3.866353	2.173719	5.014409
H	-2.966056	2.090133	6.545556
H	-3.662686	0.625214	5.819771
C	2.376671	1.028248	3.504116
C	3.084226	-0.114513	3.903248
C	4.427090	-0.234716	3.541877
H	4.982170	-1.115274	3.866335
C	5.072150	0.734909	2.779491
C	4.340720	1.854419	2.383678
H	4.820307	2.620389	1.775538
C	3.002612	2.020147	2.731051
C	2.403126	-1.196459	4.703719
H	2.006610	-0.819165	5.654060
H	3.098227	-2.012070	4.927401
H	1.551368	-1.619436	4.155159
C	6.513869	0.578597	2.366255
H	6.592092	0.428136	1.282358
H	6.980699	-0.281272	2.859352
H	7.102342	1.469104	2.616978
C	2.240952	3.242483	2.284046
H	1.421767	2.969207	1.606481
H	2.899999	3.932412	1.747330
H	1.793678	3.777976	3.130441
C	-3.214136	0.306391	3.158806
C	-3.963667	1.147404	2.319840
C	-5.183840	0.689294	1.828550
H	-5.762896	1.341721	1.176317
C	-5.677292	-0.576522	2.142594
C	-4.907720	-1.395646	2.964458
H	-5.273538	-2.390353	3.220610
C	-3.675142	-0.980092	3.471935
C	-3.454412	2.517946	1.951687
H	-3.141506	3.088708	2.833976
H	-4.221657	3.088573	1.421085
H	-2.584645	2.448670	1.284359
C	-7.012247	-1.029701	1.604789
H	-7.180555	-2.095515	1.794750
H	-7.077952	-0.865602	0.522212
H	-7.837383	-0.476572	2.069696
C	-2.849675	-1.899908	4.336395
H	-1.869255	-2.095938	3.882984
H	-3.354459	-2.861209	4.476233
H	-2.656542	-1.470647	5.326993
C	1.224089	3.220035	-3.935612
N	1.429685	2.676370	-2.743662
C	-0.041048	3.351740	-4.545104

H	-0.033728	3.756332	-5.550888
C	-1.314680	3.172197	-3.974431
N	-1.535750	2.681199	-2.758492
C	2.401903	3.770702	-4.715164
H	2.860436	4.604656	-4.171676
H	2.090733	4.127403	-5.698944
H	3.181260	3.012387	-4.842544
C	-2.493959	3.598199	-4.827725
H	-3.239566	2.797610	-4.879607
H	-2.173337	3.850407	-5.840566
H	-2.996979	4.470344	-4.396468
C	2.752843	2.706719	-2.201041
C	3.145877	3.796045	-1.405574
C	4.440650	3.821209	-0.892437
H	4.752851	4.677100	-0.292824
C	5.347646	2.787390	-1.132086
C	4.918504	1.701207	-1.889571
H	5.601178	0.872565	-2.076402
C	3.632730	1.640830	-2.431354
C	2.180750	4.919516	-1.119615
H	1.808981	5.386568	-2.039583
H	2.655084	5.695693	-0.510521
H	1.299943	4.555138	-0.574483
C	6.758207	2.867746	-0.601785
H	7.321329	3.667213	-1.098198
H	7.300425	1.930175	-0.765207
H	6.775005	3.078494	0.474283
C	3.203961	0.457075	-3.260115
H	2.409556	-0.106313	-2.754245
H	4.043281	-0.225113	-3.422780
H	2.810534	0.763104	-4.237020
C	-2.856163	2.792289	-2.221842
C	-3.720998	1.690726	-2.223375
C	-5.007309	1.846575	-1.700089
H	-5.681364	0.989565	-1.709740
C	-5.450918	3.056814	-1.176948
C	-4.557135	4.129317	-1.155713
H	-4.874798	5.080937	-0.728976
C	-3.263197	4.015029	-1.655914
C	-3.283164	0.360395	-2.779082
H	-2.785828	0.466690	-3.750540
H	-4.138105	-0.310758	-2.900011
H	-2.575822	-0.141836	-2.104070
C	-6.849826	3.211989	-0.632029
H	-6.837371	3.539558	0.415045
H	-7.402270	2.267371	-0.680034
H	-7.417480	3.959711	-1.198316
C	-2.307973	5.180945	-1.586058
H	-1.376573	4.895929	-1.081214
H	-2.754356	6.016130	-1.037545
H	-2.022096	5.544590	-2.580749

Model $Pd(H_2)_3$

SCF (wB97x) = -131.446063431
E(SCF)+ZPE(0 K)= -131.401728
H(298 K)= -131.396126
G(298 K)= -131.426811
Lowest Frequency = 373.0031cm-1

Pd	-0.000001	0.000015	-0.000005
H	-0.397561	-1.733209	0.000020
H	1.699744	0.522030	0.000147
H	-1.302318	1.210728	-0.000016
H	1.278194	1.236219	-0.000056
H	-1.709769	0.488396	0.000113
H	0.431753	-1.724841	0.000005

Model $[PdMg_3H_3]^{3+}$

SCF (wB97x) = -728.895201764
E(SCF)+ZPE(0 K)= -728.875630
H(298 K)= -728.866385
G(298 K)= -728.909873
Lowest Frequency = 88.5782cm-1

Pd	-0.000147	0.000030	0.000000
Mg	-2.495992	0.321035	-0.000008
Mg	0.970064	-2.321872	-0.000008
Mg	1.526174	2.000791	0.000016
H	-1.022002	-1.351105	-0.000011
H	1.680701	-0.212045	0.000006
H	-0.654877	1.562331	0.000005

1a

SCF (wB97x) = -3849.61939070
E(SCF)+ZPE(0 K)= -3847.650199
H(298 K)= -3847.539261
G(298 K)= -3847.795305
Lowest Frequency = 13.1985cm-1

Pd	-0.142429	0.035084	0.159632
Mg	0.152962	2.182314	-1.156424
Mg	1.870442	-1.344588	0.883396
Mg	-2.561638	-0.792358	0.239145

H	-0.510224	-1.476201	0.882259
H	-1.465257	0.957727	-0.416443
N	1.422945	2.604738	-2.725557
C	1.128490	3.543450	-3.616805
C	0.092111	4.486365	-3.471696
H	-0.016421	5.178176	-4.298970
C	-0.673179	4.799708	-2.328526
N	-0.757326	4.044040	-1.238078
C	1.974300	3.680755	-4.867626
H	3.003344	3.954115	-4.610706
H	1.567673	4.442600	-5.535589
H	2.026194	2.728684	-5.406371
C	-1.401281	6.130023	-2.388894
H	-2.483816	5.993932	-2.334286
H	-1.162851	6.662746	-3.311164
H	-1.121669	6.759791	-1.537692
C	2.693674	1.948436	-2.854075
C	3.810537	2.528276	-2.217430
C	5.056710	1.917848	-2.360512
H	5.927739	2.364784	-1.884519
C	5.204476	0.745779	-3.088635
H	6.183739	0.283547	-3.187191
C	4.091299	0.165815	-3.682152
H	4.203380	-0.759061	-4.245220
C	2.828399	0.752789	-3.586061
C	3.703059	3.794955	-1.377594
H	2.660136	4.129102	-1.398584
C	4.076130	3.515683	0.083939
H	3.441987	2.735586	0.524691
H	3.971431	4.424274	0.690210
H	5.116388	3.179498	0.173262
C	4.555711	4.933988	-1.949930
H	4.422534	5.847255	-1.357351
H	4.277681	5.161570	-2.985545
H	5.622999	4.681624	-1.937297
C	1.641669	0.086853	-4.264355
H	0.818678	0.808357	-4.264364
C	1.922001	-0.285003	-5.725199
H	2.285586	0.573588	-6.302316
H	1.004652	-0.651754	-6.200919
H	2.670430	-1.082236	-5.804314
C	1.187160	-1.147343	-3.474427
H	1.972794	-1.914827	-3.452883
H	0.290272	-1.593145	-3.925650
H	0.949327	-0.883786	-2.435454
C	-1.475782	4.588600	-0.120055
C	-2.884928	4.547474	-0.064079
C	-3.531603	5.224885	0.971825
H	-4.619438	5.222243	1.010396
C	-2.818765	5.887705	1.959747
H	-3.341162	6.417174	2.752749
C	-1.431365	5.834142	1.950531
H	-0.876449	6.315300	2.751391
C	-0.739084	5.181938	0.928925
C	-3.733301	3.746431	-1.045827
H	-3.066720	3.330623	-1.811306
C	-4.812927	4.579562	-1.750198
H	-5.540338	4.977039	-1.032505
H	-5.364527	3.953655	-2.462073
H	-4.398103	5.427744	-2.304198
C	-4.402819	2.574101	-0.312117
H	-3.658544	1.945530	0.189523
H	-4.973583	1.949098	-1.010221
H	-5.099840	2.937131	0.453989
C	0.785652	5.149559	0.949163
H	1.107558	4.236740	0.430153
C	1.359824	5.075919	2.367932
H	1.247745	6.025959	2.904397
H	2.430144	4.844874	2.329233
H	0.870027	4.289772	2.953229
C	1.387575	6.337459	0.187062
H	1.111515	6.322395	-0.873050
H	2.482989	6.318591	0.247337
H	1.041940	7.285042	0.619356
N	3.071671	-1.205260	2.559969
C	3.302479	-2.298478	3.268785
C	3.062444	-3.607440	2.797631
H	3.231284	-4.398226	3.519686
C	2.864191	-4.037417	1.469019
N	2.616803	-3.233190	0.438511
C	3.900047	-2.181760	4.655011
H	4.920874	-1.787873	4.593881
H	3.933383	-3.152361	5.153995
H	3.326517	-1.482392	5.271464
C	2.977261	-5.533604	1.247592
H	1.993871	-5.949987	1.006142
H	3.352953	-6.035594	2.141369
H	3.638829	-5.764390	0.407920
C	3.550435	0.058823	3.036202
C	4.842057	0.488218	2.669588
C	5.256904	1.766679	3.046285
H	6.250387	2.109632	2.762309
C	4.425240	2.609948	3.770769
H	4.761324	3.606129	4.048968
C	3.167285	2.163227	4.152793
H	2.522578	2.816544	4.737890

C	2.714707	0.888169	3.808630
C	5.794334	-0.396467	1.877200
H	5.304030	-1.362315	1.713007
C	6.088692	0.211510	0.503057
H	5.169982	0.363339	-0.075037
H	6.752607	-0.441219	-0.077196
H	6.583790	1.186609	0.599780
C	7.097459	-0.661654	2.641307
H	7.667622	0.262565	2.795070
H	7.734499	-1.355618	2.079461
H	6.906364	-1.101344	3.626885
C	1.346282	0.429140	4.283441
H	1.226004	-0.626673	4.014507
C	1.205237	0.535453	5.807572
H	1.998923	-0.010143	6.331811
H	0.239639	0.123507	6.121902
H	1.246133	1.579542	6.141143
C	0.222209	1.202702	3.592819
H	0.238873	2.263450	3.879188
H	-0.747370	0.786938	3.881662
H	0.302076	1.144191	2.498243
C	2.672513	-3.787850	-0.883939
C	1.537265	-4.388497	-1.459523
C	1.628334	-4.907693	-2.753695
H	0.751896	-5.368308	-3.205125
C	2.811418	-4.845860	-3.469983
H	2.869904	-5.261239	-4.473009
C	3.923908	-4.237359	-2.900074
H	4.842469	-4.184331	-3.476365
C	3.881048	-3.691969	-1.615892
C	0.200432	-4.471235	-0.739470
H	0.331313	-4.083259	0.277162
C	-0.314690	-5.913143	-0.633948
H	-0.532032	-6.334281	-1.623064
H	-1.245605	-5.945835	-0.054185
H	0.409787	-6.576962	-0.149873
C	-0.836554	-3.587593	-1.440241
H	-0.488004	-2.553050	-1.519459
H	-1.777463	-3.588236	-0.874027
H	-1.059268	-3.948261	-2.452525
C	5.115512	-3.002454	-1.035772
H	4.765192	-2.087535	-0.538129
C	6.127878	-2.591375	-2.109386
H	6.897829	-1.948779	-1.668361
H	6.640782	-3.464320	-2.531962
H	5.654916	-2.040167	-2.927049
C	5.847342	-3.850472	0.016511
H	6.768081	-3.341160	0.329588
H	5.249338	-4.020245	0.915093
H	6.131346	-4.823899	-0.403809
N	-3.852474	-0.978733	1.854083
C	-5.168304	-1.005428	1.719392
C	-5.841531	-0.870142	0.485626
H	-6.917073	-0.751583	0.561310
C	-5.343042	-1.007132	-0.817001
N	-4.070096	-1.264462	-1.127381
C	-6.068968	-1.183208	2.928127
H	-5.641448	-1.895977	3.638760
H	-7.053439	-1.539538	2.617262
H	-6.204788	-0.236455	3.461176
C	-6.372377	-0.836868	-1.921352
H	-6.245865	0.158365	-2.364891
H	-7.389025	-0.901033	-1.527067
H	-6.257229	-1.566394	-2.725388
C	-3.298841	-1.053662	3.172095
C	-2.620270	-2.228211	3.561645
C	-2.087996	-2.292262	4.850265
H	-1.569904	-3.190305	5.174603
C	-2.214161	-1.227642	5.734169
H	-1.805777	-1.302561	6.739386
C	-2.854074	-0.065913	5.325125
H	-2.924539	0.773248	6.013684
C	-3.396413	0.051381	4.043814
C	-2.505738	-3.420657	2.618054
H	-2.391899	-3.029141	1.598909
C	-1.276052	-4.292917	2.883479
H	-1.356973	-4.838034	3.831690
H	-0.355177	-3.697078	2.906652
H	-1.175639	-5.042904	2.089949
C	-3.781759	-4.272939	2.629780
H	-3.967381	-4.678902	3.632067
H	-3.684116	-5.116887	1.934313
H	-4.659161	-3.690576	2.327974
C	-4.025889	1.375047	3.619179
H	-4.621145	1.203668	2.716848
C	-4.961566	1.957996	4.686223
H	-5.701614	1.226782	5.031897
H	-5.498471	2.823506	4.281424
H	-4.405234	2.305284	5.564711
C	-2.951747	2.404903	3.248401
H	-2.319983	2.639664	4.114032
H	-3.415836	3.335951	2.906010
H	-2.297588	2.041930	2.446099
C	-3.814770	-1.778312	-2.443199
C	-3.388884	-0.939270	-3.489863
C	-3.147153	-1.501194	-4.747423

H	-2.822542	-0.858444	-5.563741
C	-3.331669	-2.854647	-4.979831
H	-3.148773	-3.272117	-5.966843
C	-3.755831	-3.675201	-3.940732
H	-3.895107	-4.736632	-4.129093
C	-3.995462	-3.166687	-2.664745
C	-3.210467	0.562717	-3.316556
H	-3.404609	0.805967	-2.266502
C	-4.195461	1.361089	-4.181142
H	-4.012870	1.187119	-5.248641
H	-4.080174	2.436924	-3.996829
H	-5.236514	1.088603	-3.977477
C	-1.775752	0.990553	-3.635544
H	-1.062848	0.417353	-3.033508
H	-1.635071	2.064835	-3.445091
H	-1.531240	0.818501	-4.691764
C	-4.450534	-4.109421	-1.549977
H	-4.089122	-3.691246	-0.600538
C	-3.880299	-5.526664	-1.692642
H	-4.387344	-6.085309	-2.488992
H	-4.037481	-6.084288	-0.761416
H	-2.809106	-5.523546	-1.911578
C	-5.980973	-4.217373	-1.450412
H	-6.449372	-3.283591	-1.131963
H	-6.252949	-4.986206	-0.716980
H	-6.408765	-4.508671	-2.418135
H	1.480880	0.548380	-0.055641

Model $[Pd(PH_3)Mg_2H_2]^{2+}$

SCF (wB97x) = -871.878093735
E(SCF)+ZPE(0 K)= -871.833501
H(298 K)= -871.824309
G(298 K)= -871.868343
Lowest Frequency = 51.3135cm-1

Pd	-0.000970	-0.007481	0.143312
H	0.913014	1.368101	0.273623
H	-0.917268	-1.385135	0.198034
Mg	-0.912340	-1.398960	-1.702875
Mg	0.968919	1.435872	-1.630385
P	-0.019235	-0.015558	2.504208
H	-0.564378	1.131015	3.093704
H	-0.712511	-1.043187	3.151158
H	1.244770	-0.084668	3.101683

2c

SCF (wB97x) = -3647.61346572
E(SCF)+ZPE(0 K)= -3645.803253
H(298 K)= -3645.708047
G(298 K)= -3645.933277
Lowest Frequency = 14.2161cm-1

Pt	12.552287	3.456191	3.324838
Mg	14.172495	5.440288	2.800743
Mg	10.880824	4.766934	1.788200
P	12.561997	1.435205	4.610838
N	16.068425	5.196498	1.974262
C	16.769994	6.214291	1.490755
C	16.469286	7.571708	1.712077
H	17.158272	8.275760	1.259104
C	15.527938	8.135398	2.592877
N	14.528757	7.469779	3.164309
C	18.038581	5.952573	0.700708
H	18.842162	5.611350	1.363042
H	18.374061	6.860293	0.194460
H	17.885403	5.163787	-0.041798
C	15.726338	9.610024	2.892598
H	14.888231	10.206575	2.519748
H	16.644974	9.979869	2.433587
H	15.780195	9.781864	3.972639
C	16.707512	3.911680	1.945755
C	17.656337	3.606854	2.947980
C	18.335831	2.392074	2.882481
H	19.078888	2.153144	3.641026
C	18.077912	1.475449	1.870153
H	18.623962	0.535862	1.829700
C	17.108480	1.763741	0.922680
H	16.894012	1.039692	0.138965
C	16.411453	2.975772	0.939464
C	17.930125	4.550597	4.113546
H	17.461676	5.515596	3.892472
C	17.279495	4.007086	5.393043
H	16.198095	3.874045	5.261268
H	17.442287	4.694002	6.233711
H	17.707842	3.033736	5.666859
C	19.424187	4.810296	4.337823
H	19.953205	3.903756	4.654822
H	19.562324	5.562102	5.123750
H	19.910761	5.179714	3.427846
C	15.374179	3.236973	-0.139891
H	14.968303	4.242476	0.014892
C	15.991805	3.202414	-1.543387
H	16.808183	3.928124	-1.643228
H	15.230566	3.438559	-2.294968

H	16.398358	2.210903	-1.777826
C	14.209621	2.245809	-0.025982
H	14.552011	1.212057	-0.171535
H	13.450492	2.463456	-0.786202
H	13.735791	2.316790	0.962202
C	13.743816	8.175792	4.135824
C	12.698884	9.036571	3.735653
C	11.990411	9.732820	4.716529
H	11.184734	10.401116	4.418525
C	12.303826	9.604783	6.063675
H	11.752859	10.170630	6.810970
C	13.316667	8.737130	6.447247
H	13.551615	8.624223	7.503762
C	14.034733	7.998352	5.504494
C	12.313863	9.224731	2.273253
H	13.093087	8.763968	1.656533
C	12.201154	10.700061	1.866585
H	12.045289	10.780598	0.784330
H	13.100191	11.271014	2.123581
H	11.349871	11.188165	2.355454
C	10.998067	8.504009	1.963782
H	11.071913	7.435497	2.198853
H	10.726079	8.601704	0.906357
H	10.172417	8.911363	2.561652
C	15.114886	7.039067	5.988460
H	15.488446	6.482687	5.121091
C	14.549222	6.017997	6.983749
H	14.176107	6.504146	7.893397
H	15.326126	5.304746	7.283653
H	13.723469	5.451863	6.536851
C	16.309256	7.794381	6.583853
H	16.747588	8.484658	5.853528
H	17.092079	7.092534	6.897158
H	16.011499	8.379262	7.462941
N	8.959423	5.308359	2.388464
C	8.203897	6.152847	1.697618
C	8.482666	6.586463	0.387565
H	7.762342	7.279071	-0.032518
C	9.447854	6.104618	-0.515967
N	10.469442	5.317386	-0.190988
C	6.912218	6.675880	2.297744
H	6.209829	5.857288	2.487437
H	6.434780	7.397657	1.632097
H	7.101549	7.157160	3.263192
C	9.243522	6.530538	-1.959200
H	10.030576	7.221156	-2.277902
H	8.280215	7.028874	-2.083029
H	9.282620	5.669900	-2.634023
C	8.368646	4.741700	3.567525
C	7.610885	3.559243	3.440362
C	6.971290	3.045275	4.569833
H	6.372003	2.141012	4.478981
C	7.070447	3.677970	5.801460
H	6.542708	3.281654	6.665869
C	7.855783	4.816927	5.923469
H	7.948439	5.299829	6.894275
C	8.520385	5.361148	4.823082
C	7.456691	2.836421	2.108160
H	7.976925	3.422667	1.343210
C	8.117435	1.453155	2.157270
H	9.188826	1.541385	2.375311
H	8.003071	0.936384	1.195311
H	7.664269	0.820558	2.931645
C	5.988827	2.726976	1.678294
H	5.407204	2.115227	2.378521
H	5.914453	2.260433	0.688448
H	5.514380	3.713399	1.621562
C	9.408953	6.580183	5.008705
H	9.656432	6.968169	4.015235
C	8.730111	7.712703	5.786596
H	7.777437	8.008131	5.330560
H	9.386871	8.590329	5.810388
H	8.527975	7.427819	6.826147
C	10.723491	6.171336	5.684345
H	10.535021	5.783885	6.695455
H	11.396652	7.030422	5.770936
H	11.236803	5.388741	5.109087
C	11.259526	4.795616	-1.268385
C	12.263749	5.574477	-1.879012
C	12.964849	5.035262	-2.959863
H	13.740094	5.627704	-3.441636
C	12.685090	3.764042	-3.439838
H	13.229166	3.368613	-4.294227
C	11.717985	2.992236	-2.808908
H	11.522067	1.987694	-3.173741
C	11.007453	3.477731	-1.710248
C	12.619868	6.974995	-1.395925
H	11.839220	7.303281	-0.701020
C	12.700500	8.000916	-2.534351
H	13.561395	7.811517	-3.186147
H	12.820389	9.010002	-2.122857
H	11.803537	7.993883	-3.163482
C	13.942544	6.958037	-0.623429
H	14.765717	6.592832	-1.251276
H	13.879684	6.293681	0.246274
H	14.210671	7.958853	-0.265667

C	9.967516	2.597801	-1.024541
H	9.941668	2.880237	0.035758
C	10.318416	1.107937	-1.075478
H	10.217360	0.695560	-2.086710
H	9.638831	0.543366	-0.427574
H	11.343097	0.925757	-0.730157
C	8.560279	2.833794	-1.589033
H	8.227353	3.865601	-1.433623
H	7.834770	2.172250	-1.098221
H	8.535965	2.622036	-2.665549
C	14.255990	0.846553	5.166566
H	14.762640	1.792687	5.412569
C	15.052864	0.209469	4.014686
H	15.067024	0.881688	3.145666
H	14.559277	-0.720069	3.697966
C	16.485804	-0.129162	4.435290
H	17.011653	-0.600590	3.596164
H	17.024187	0.803202	4.652774
C	16.516380	-1.029328	5.668498
H	17.551766	-1.241425	5.963061
H	16.050020	-1.997576	5.430973
C	15.757339	-0.371581	6.818602
H	16.272119	0.558233	7.104740
H	15.757518	-1.017844	7.705333
C	14.313821	-0.043752	6.423606
H	13.772011	-0.982781	6.249459
H	13.824703	0.448733	7.270798
C	11.662968	0.018587	3.794660
H	10.630562	0.401412	3.787772
C	12.031837	-0.187099	2.314249
H	13.064470	-0.548475	2.221437
H	11.986008	0.774589	1.789514
C	11.088828	-1.197866	1.652058
H	10.071181	-0.778755	1.629732
H	11.385966	-1.353711	0.607114
C	11.062399	-2.529791	2.403721
H	10.356642	-3.222800	1.929254
H	12.055357	-3.000326	2.344793
C	10.694824	-2.318653	3.873125
H	10.710105	-3.272927	4.414375
H	9.665921	-1.933576	3.938446
C	11.646417	-1.322708	4.544379
H	12.657502	-1.753829	4.551133
H	11.354776	-1.181043	5.593151
C	11.670236	1.599308	6.234937
H	11.836977	0.665301	6.790177
C	10.149430	1.777570	6.115756
H	9.920536	2.701698	5.565502
H	9.698426	0.952707	5.550062
C	9.516274	1.826669	7.510779
H	8.431484	1.950153	7.418552
H	9.684333	0.862319	8.015008
C	10.107868	2.950633	8.362194
H	9.667851	2.941571	9.367493
H	9.842696	3.915313	7.906281
C	11.631345	2.837692	8.447756
H	12.048007	3.692946	8.995225
H	11.897574	1.936312	9.021136
C	12.264428	2.756985	7.056031
H	13.354386	2.659494	7.148709
H	12.085479	3.693657	6.511837
H	13.894958	3.991631	4.148476
H	11.204870	2.937534	2.501570

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