

A low-valent lead hydride and its extreme low-field ^1H NMR chemical shift

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1. General Details

General procedures: All manipulations were carried out under argon atmosphere using standard Schlenk techniques or an MBraun Glovebox. Benzene was distilled from sodium/benzophenone, toluene from sodium. Hexane and pentane were obtained from an MBRAUN solvent purification system and degassed by three cycles of freeze-pump-thaw. Catecholborane was purchased from Alfa Aesar, used as received after degassing by three cycles of freeze-pump thaw and stored in a freezer of an MBraun Glovebox. ^{Me}NHC was prepared according to literature procedures.¹ The deuterated catecholborane was generated according to the literature procedure of Brown for the synthesis of the non-deuterated catecholborane with few modifications.² Elemental analysis was performed by the Institut für Anorganische Chemie, Universität Tübingen using a Vario MICRO EL analyzer. IR spectra were recorded as KBr pellets prepared in a glovebox and measured with a Bruker VERTEX 70 IR spectrometer.

NMR spectroscopy: NMR spectra were recorded with either a Bruker DRX-250 NMR spectrometer equipped with a 5 mm ATM probe head and operating at 250.13 (¹H), 62.90 (¹³C), 101.25 (³¹P), 80.25 (¹¹B) and 52.33 MHz (²⁰⁷Pb), a Bruker Avance⁺400 NMR spectrometer equipped with a 5 mm QNP (quad nucleus probe) head and operating at 400.13 (¹H), 100.62 (¹³C), 161.97 (³¹P) or a Bruker AVII+ 500 NMR spectrometer with a variable temperature set up and a 5 mm ATM or a 5 mm TBO probe head and operating at 500.13 (¹H), 125.76 (¹³C), 202.46 (³¹P), 160.46 (¹¹B) and 104.63 MHz (²⁰⁷Pb). Chemical shifts are reported in δ values in ppm relative to external SiMe₄ (¹H, ¹³C), aqueous 85% H₃PO₄ (³¹P), BF₃ · Et₂O (¹¹B), or PbMe₄ (²⁰⁷Pb) using the chemical shift of the solvent ²H resonance and the following frequency ratios $\Xi = 25.145020\%$ for ¹³C, 40.480742% for ³¹P, 32.083974% for ¹¹B and 20.920599% for ²⁰⁷Pb.³ H-1 solid state MAS NMR spectra of **2** were obtained on a Bruker AVII+500 standard bore spectrometer using a 2.5 mm MAS broad band probe head. A powdered sample of **2** was placed in a 2.5 mm o.d. zirconia rotor and MAS NMR spectra were obtained at spinning rates between 15 and 25 kHz. Chemical shifts are referenced to external 1% TMS in CDCl₃. Typical parameters: 200 scans, recycle delay 4 s, 2 μ s 90° pulse. Because of the low intensities of the spinning sidebands only the span $\Omega = \delta_{11} - \delta_{33}$ of the hydride ¹H NMR chemical shift tensor can be estimated, $\Omega = 100 \pm 10$ ppm, whereas the skew is ill-defined.

2. Experimental and spectroscopic data of lead hydride **2**

In a J. Young NMR tube plumbylene **1**⁴ (15.4 mg, 16.0 μ mol, 1 eq) was dissolved in 0.5 mL of C₆D₆ and catecholborane (1.74 μ L, 16.0 μ mol, 1 eq) was added via a micropipette at ambient temperature. Within three minutes, the dark purple solution turned yellow and subsequently recorded ¹H and ³¹P{¹H} NMR spectra showed quantitative formation of the terphenyl-substituted lead hydride **2** and

phosphine **3**. Within 0.5 hours, elemental lead was visible and in the ^1H NMR spectra the decomposition of the lead hydride got obvious through the decrease of the intensity of the hydride signal and increase of signals corresponding to Powers diplumbyne. At the same time a signal at 4.45 ppm hints towards hydrogen release. Within 2.5 hours at RT the hydride signal completely vanished. Therefore, the reaction protocol was adjusted in terms of the reaction temperature and plumbylene **1** (72.8 mg, 75.5 μmol , 1 eq) was dissolved in 1.7 mL toluene and cooled to -40°C . To the precooled solution catecholborane (8.22 μL , 75.5 μmol , 1 eq) was added via a micropipette and the reaction mixture was stored for ca. 20 minutes at -40°C until the dark purple solution turned yellow-orange. The solution was reduced to ca. 1 mL *in vacuo* and layered with 0.7 mL of *n*-hexane and stored at -40°C . Overnight, yellow crystals suitable for single crystal X-ray crystallography could be obtained. However, besides the yellow crystals of the lead hydride, the boryl phosphine **3** precipitated as colorless powder. By fractional crystallization, a small amount of pure lead hydride crystals could be obtained (7.5 mg, 10.9 μmol , 14%). The yields were variable for different experiments, but up to 55% of pure hydride could be obtained after combining three fractions of crystals.

^1H (500.13 MHz, Tol-d8, 26 $^\circ\text{C}$): δ (ppm) 1.10 (d, $^3J_{\text{HH}} = 6.7$ Hz, 24H, $\text{CH}_3\text{-iPr}$), 1.12 (d, $^3J_{\text{HH}} = 7.0$ Hz, 24H, $\text{CH}_3\text{-iPr}$), 1.40 (d, $^3J_{\text{HH}} = 6.8$ Hz, 24H, $\text{CH}_3\text{-iPr}$), 2.98, (sept., $^3J_{\text{HH}} = 6.8$ Hz, 4H, $\text{CH}\text{-iPr}$), 3.05 (sept., $^3J_{\text{HH}} = 6.8$ Hz, 8H, $\text{CH}\text{-iPr}$), 7.12 (s, 8H, *m*-CH-Trip), 7.22 (t, $^3J_{\text{HH}} = 7.5$ Hz, 2H, *p*- C_6H_3), 7.49 (d, $^3J_{\text{HH}} = 7.6$ Hz, 4H, *m*- C_6H_3), 35.61 (s, $^1J_{^{207}\text{PbH}} = 734$ Hz, 2H, PbH). $^{13}\text{C}\{\text{H}\}$ (125.76 MHz, Tol-d8, -42°C): δ (ppm) 24.2-24.4 ($\text{CH}_3\text{-iPr}$, overlapped by signals of diplumbyne), 26.1 ($\text{CH}_3\text{-iPr}$), 30.6, 34.6 ($\text{CH}\text{-iPr}$), 121.3 (br s, *m*-CH-Trip), 126.0 (*p*- C_6H_3), 133.3 (*m*- C_6H_3), 139.1 (*i*-C_q-Trip), 146.0, 147.7 (*o/p*-C_q-Trip), 149.3 (*o*-C_q- C_6H_3). The *ipso*- C_6H_3 could not be identified due to the signal to noise ratio of the recorded spectrum. ^1H - ^{207}Pb HMQC (500.13 MHz, Tol-d8, -80°C): δ (ppm) 3736 (major isomer), 4400 (minor isomer). Direct detection of the ^1H decoupled as well as ^1H coupled ^{207}Pb NMR signal remained unsuccessful. Anal. Calcd. for $\text{C}_{36}\text{H}_{50}\text{Pb} \cdot 0.5$ eq C_6H_{14} : C 63.90%, H 7.84%. Found: 64.16%, H 7.27%.

A crystalline sample of $[\text{Ar}^*\text{Pb}(\mu\text{-H})]_2$ ($\text{Ar}^* = \text{C}_6\text{H}_3\text{-2,6-Trip}_2$; Trip = $\text{C}_6\text{H}_2\text{-2,4,6-iPr}_3$) was heated to determine the melting or decomposition point. Above 40°C the yellow crystals started to turn green and at 60°C the color change was completed. Between 60 and 70°C the sample color turned light grey and ultimately dark grey from 70 to 80°C, which most likely marks the decomposition point.

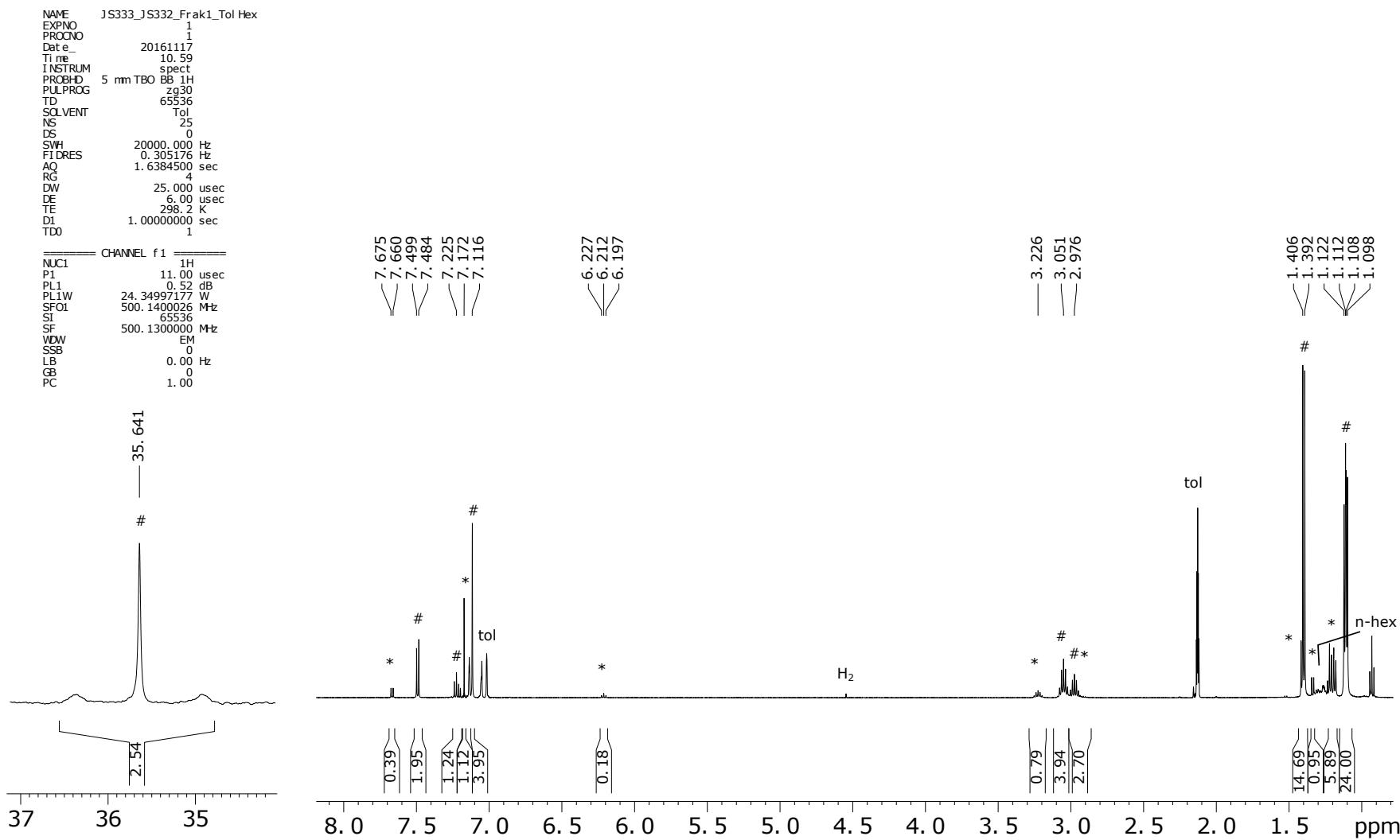


Figure SI1. ^1H NMR spectrum of **2** at ambient temperature of a crystalline sample. (# signals of **2** and * = signals of diplumbyne)

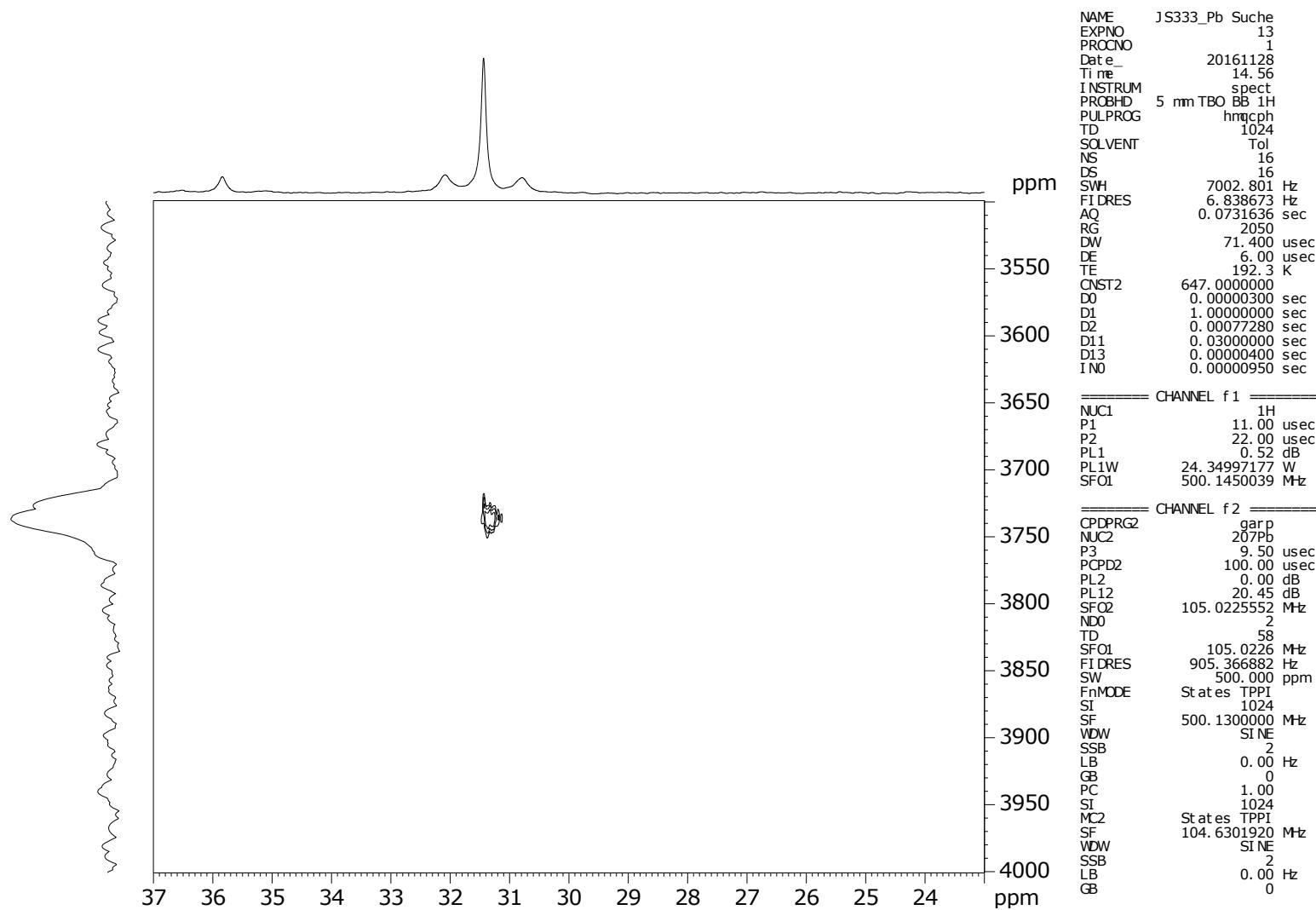


Figure SI2. ^1H - ^{207}Pb HMQC NMR spectrum of the major isomer of **2** at -80°C .

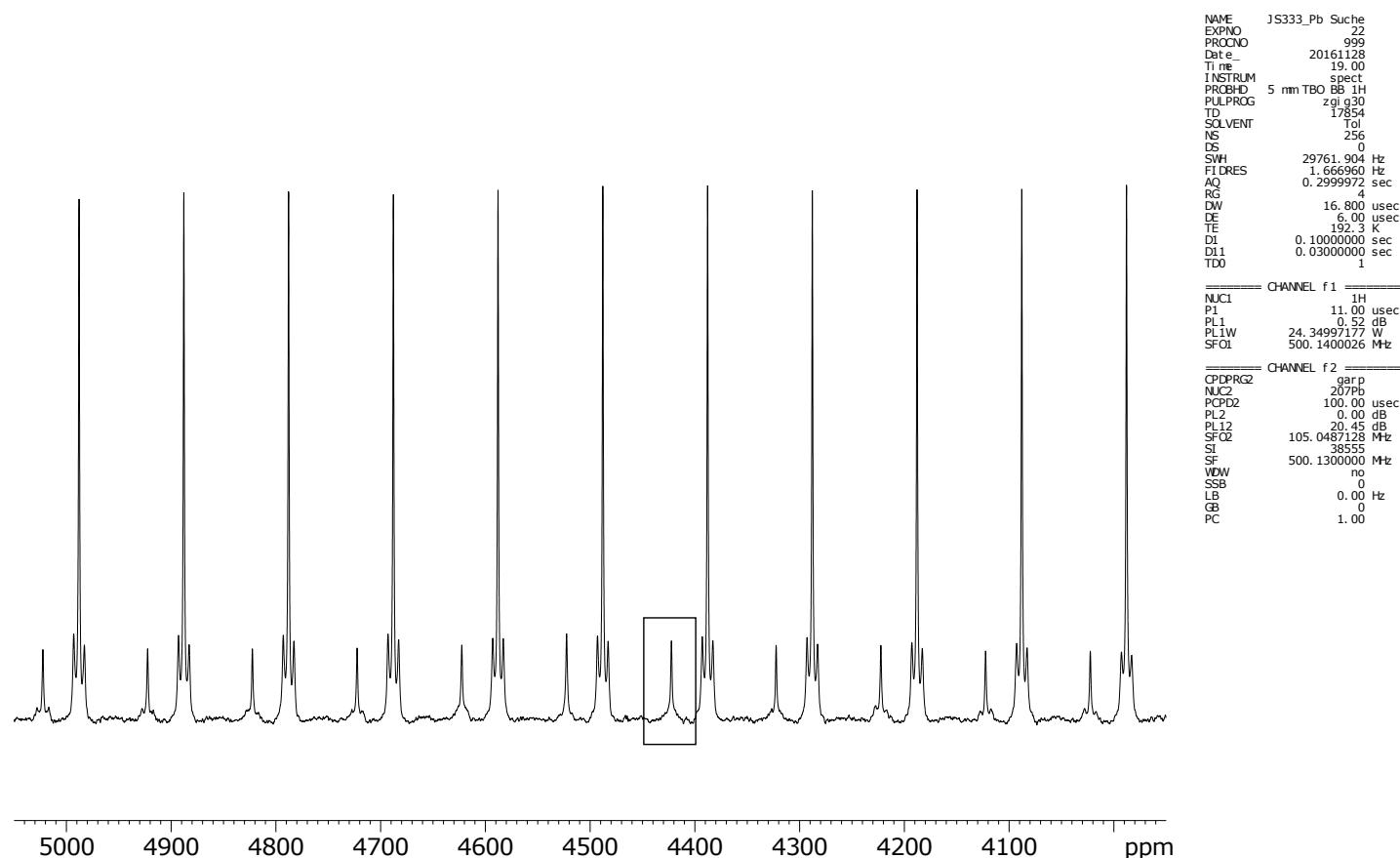


Figure SI3. ${}^1\text{H}\{\text{sel. } {}^{207}\text{Pb}\}$ -NMR experiment at -80°C for the minor isomer. The ${}^1\text{H}$ hydride region is plotted against the position of the ${}^{207}\text{Pb}$ transmitter, varied between 5000 to 4000 ppm in hundred ppm steps. Disappearance of the ${}^{207}\text{Pb}$ satellites indicates that the position of the ${}^{207}\text{Pb}$ transmitter corresponds to the ${}^{207}\text{Pb}$ chemical shift of that species.

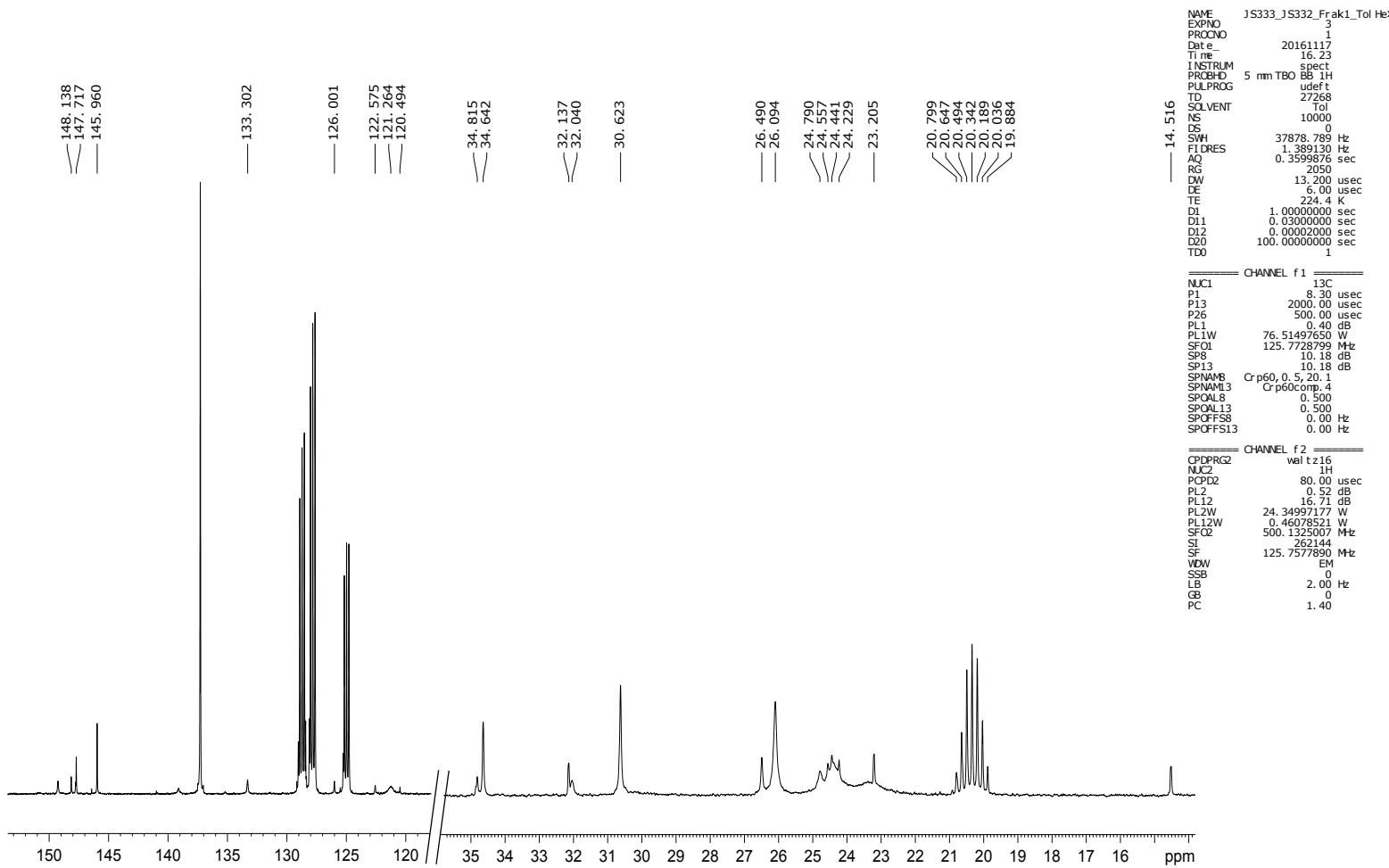


Figure SI4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum at -40°C of a crystalline sample of $[\text{Ar}^*\text{PbH}]_2$ (**2**). Small amounts of $[\text{Ar}^*\text{Pb}]_2$ can be detected due to decomposition.

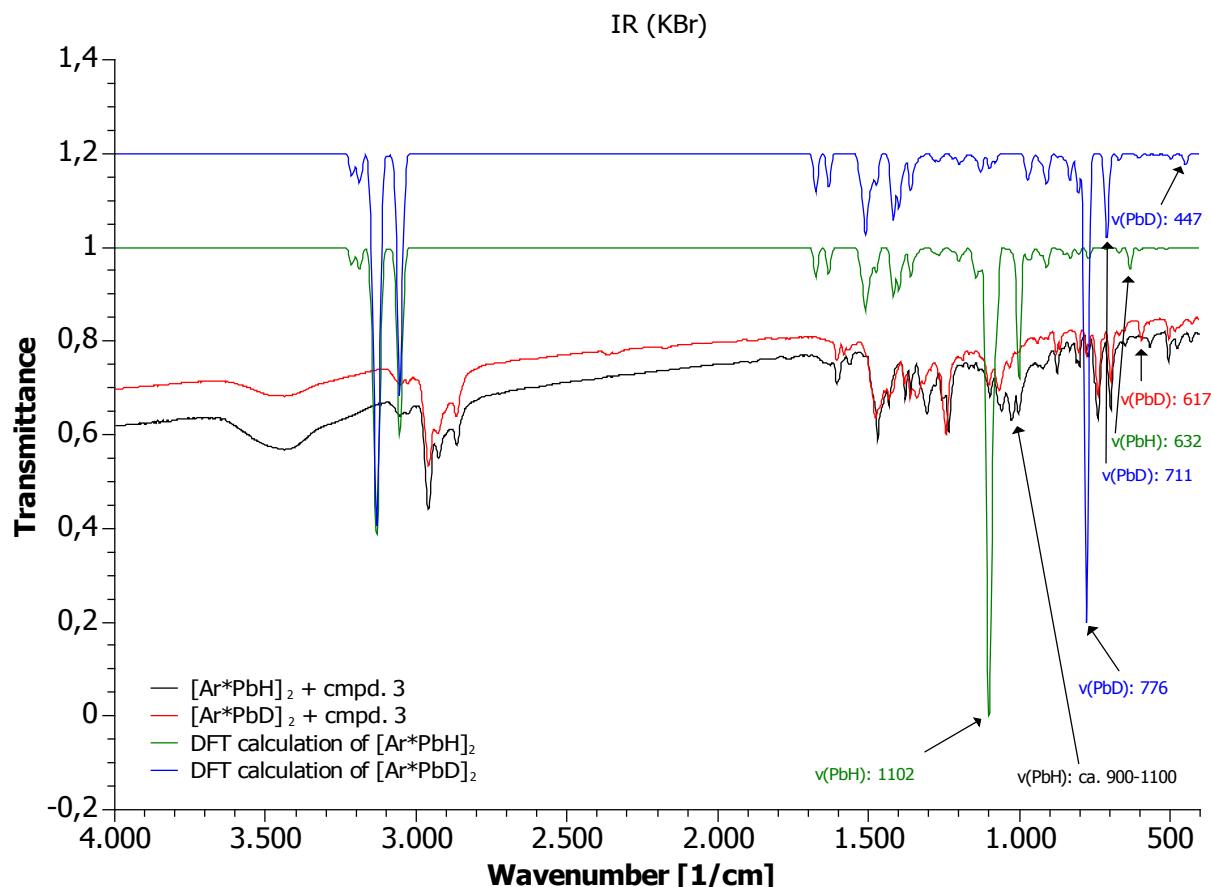


Figure SI5. Comparison of IR spectra of the reaction mixtures of lead hydride **2** or **2-D** and boryl-phosphinylmethane **3** with IR spectra calculated for **2** or **2-D**.

N. B. The deuteride compound was generated *in situ* along the lines of the hydride **2** procedure using an *in situ* prepared solution of catB-D in thf without further purification.² The IR was taken of the reaction mixture after removal of all volatiles.

Compared to the experimental IR spectra, the bands predicted by the DFT calculations appear at wavenumbers that are higher by about 100 cm⁻¹. In the region of 900-1100 cm⁻¹ the IR spectrum of the crude reaction mixture of lead hydride dimer **2** and boryl-phosphinylmethane **3** shows several PbH bands which cannot be detected in the spectrum of the reaction mixture of the respective deuteride. The DFT calculation on the lead hydride dimer **2** forecasts the PbH bands in approximately the same region. The spectrum of the reaction mixture of the deuteride and compound **3** reveals a PbD band at 617 cm⁻¹ which is not present in the spectrum of the hydride. However, the symmetric stretching band of PbD is overlapped by other bands.

3. NMR spectroscopic data of boryl-phosphinylmethane 3

¹H (500.13 MHz, C₆D₆, 26 °C): δ (ppm) 3.98 (d, ²J_{PH} = 3.1 Hz, CatBCHPh), 6.62, 6.84 (m, 2H, CH-Cat), 6.88-6.98 (m, 6H, *p*-CH-PPh₂(2H), *p*-CH-Ph (1H), *m*-CH-PPh₂ (4H)), 7.04-7.11 (m, 2H, *m*-CH-Ph), 7.33-7.38 (m, 2H, *o*-CH-PPh₂), 7.55-7.60 (m, 4H, *o*-CH-Ph, *o*-CH-PPh₂). ¹³C{¹H} (125.76 MHz, C₆D₆, 26 °C): δ (ppm) 36.0 (d, ²J_{31PC} = 16.7 Hz, CatBCHPh), 112.3, 122.5 (CatCH), 125.9 (d, ⁵J_{31PC} = 2.5 Hz, *p*-CH-Ph), 128.1-128.4 (m, *p/m*-CH-PPh₂), 128.6 (*m*-CH-Ph), 128.9 (*p*-CH-PPh₂), 129.8 (d, ³J_{31PC} = 8.8 Hz, *o*-CH-Ph), 132.8 (d, ³J_{31PC} = 19.0 Hz, *o*-CH-PPh₂), 133.4 (d, ³J_{31PC} = 20.7 Hz, *o*-CH-PPh₂), 137.8-138.1 (m, *i*-C_q-Ph/PPh₂), 148.1 (s, C_q-Cat). ³¹P{¹H} (101.25 MHz, C₆D₆, 26 °C): δ (ppm) -1.20. ¹¹B{¹H} (160.46 MHz, C₆D₆, 26 °C): δ (ppm) 33.8. Anal. Calcd. for C₂₅H₂₀BO₂P: C 76.17%, H 5.11%. Found: 76.08%, H 5.26%.

4. Experimental and spectroscopic data of ^{Me}NHC adduct 5

Lead hydride **2** (9.2 mg, 13.3 μmol, 1 eq) was dissolved in 0.2 mL toluene-d8 and a toluene-d8 solution (0.3mL) of ^{Me}NHC (2.5 mg, 20.1 3 μmol, 1.5 eq) was added. The yellow color of the solution was retained, however after 15 minutes ¹H-NMR data showed no hydride signal at 35.61 ppm and instead a new hydride signal at 23.81 ppm. Using one equivalent of ^{Me}NHC small amounts of the lead hydride dimer **2** are observed indicating the existence of an equilibrium.

¹H (400.11 MHz, Tol-d8, 26 °C): δ (ppm) 1.12 (d, ³J_{HH} = 6.8 Hz, 6H, CH₃-iPr), 1.21 (d, ³J_{HH} = 6.7 Hz, 6H, CH₃-iPr), 1.29 (d, ³J_{HH} = 6.8 Hz, 6H, CH₃-iPr), 1.32 (d, ³J_{HH} = 6.9 Hz, 6H, CH₃-iPr), 1.33 (d, ³J_{HH} = 6.9 Hz, 6H, CH₃-iPr), 1.41 (s, 6H, CH₃-^{Me}NHC), 1.64 (d, ³J_{HH} = 6.9 Hz, 6H, CH₃-iPr), 2.91 (sept., ³J_{HH} = 6.9 Hz, 2H, CH-iPr), 3.04 (sept., ³J_{HH} = 6.6 Hz, 2H, CH-iPr), 3.05 (s, 6H, NCH₃-^{Me}NHC), 3.50 (sept., ³J_{HH} = 6.6 Hz, 2H, CH-iPr), 7.02, 7.03, 7.22, 7.23 (s, 1H, CH-Trip), 7.24-7.30 (m, 3H, C₆H₃), 23.81 (s, ¹J_{PbH} = 955 Hz, 1H, PbH). ¹H-²⁰⁷Pb HMQC (500.13 MHz, C₆D₆, 26 °C): δ (ppm) 834. Direct detection of the ¹H decoupled as well as ¹H coupled ²⁰⁷Pb NMR signal remained unsuccessful.

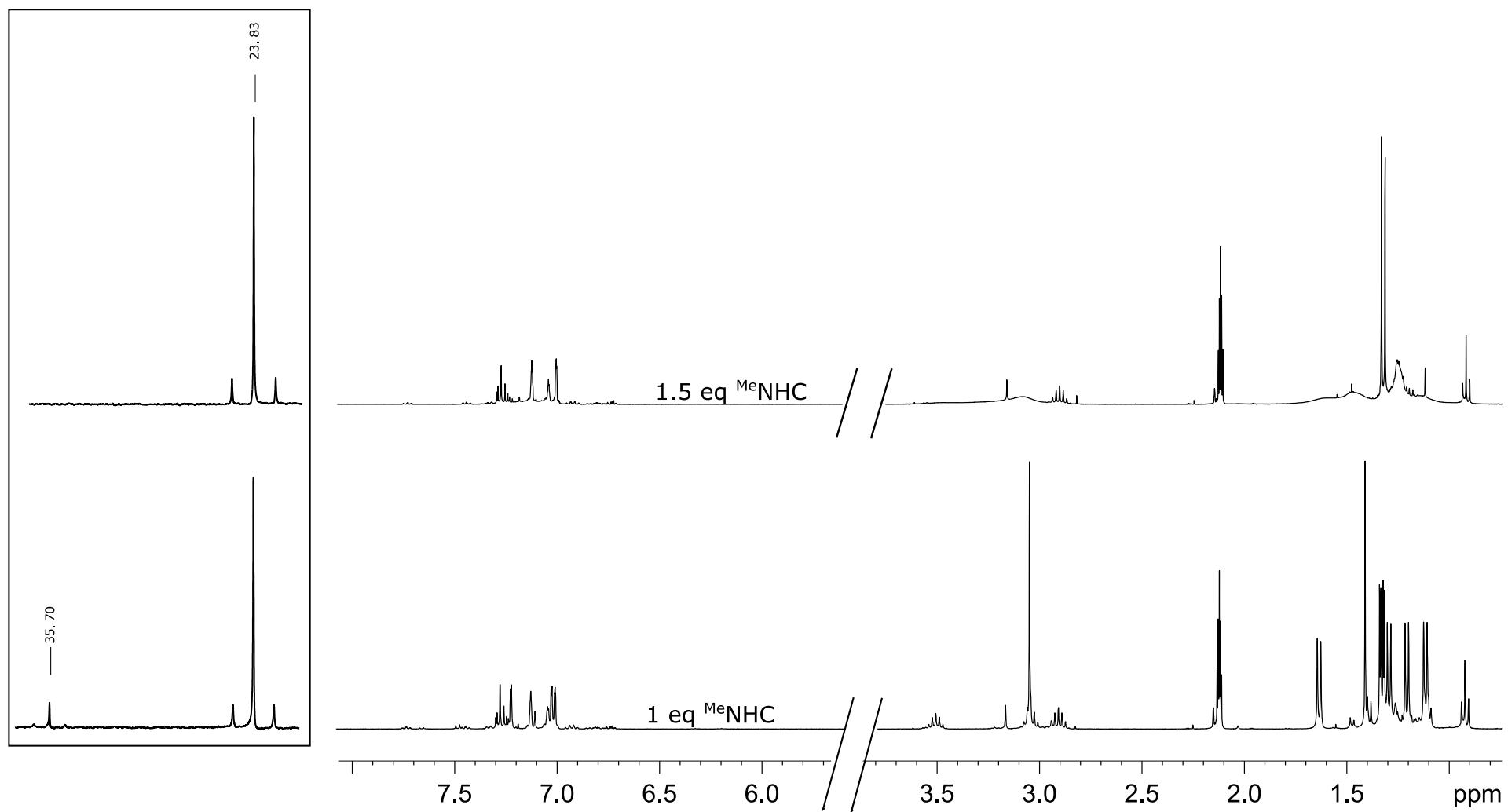


Figure SI6. ¹H NMR spectrum of a crude reaction mixture of [Ar*PbH(^{Me}NHC)] (**5**) with different equivalents of ^{Me}NHC (Tol-d₈, 400.11 MHz, 26°C).

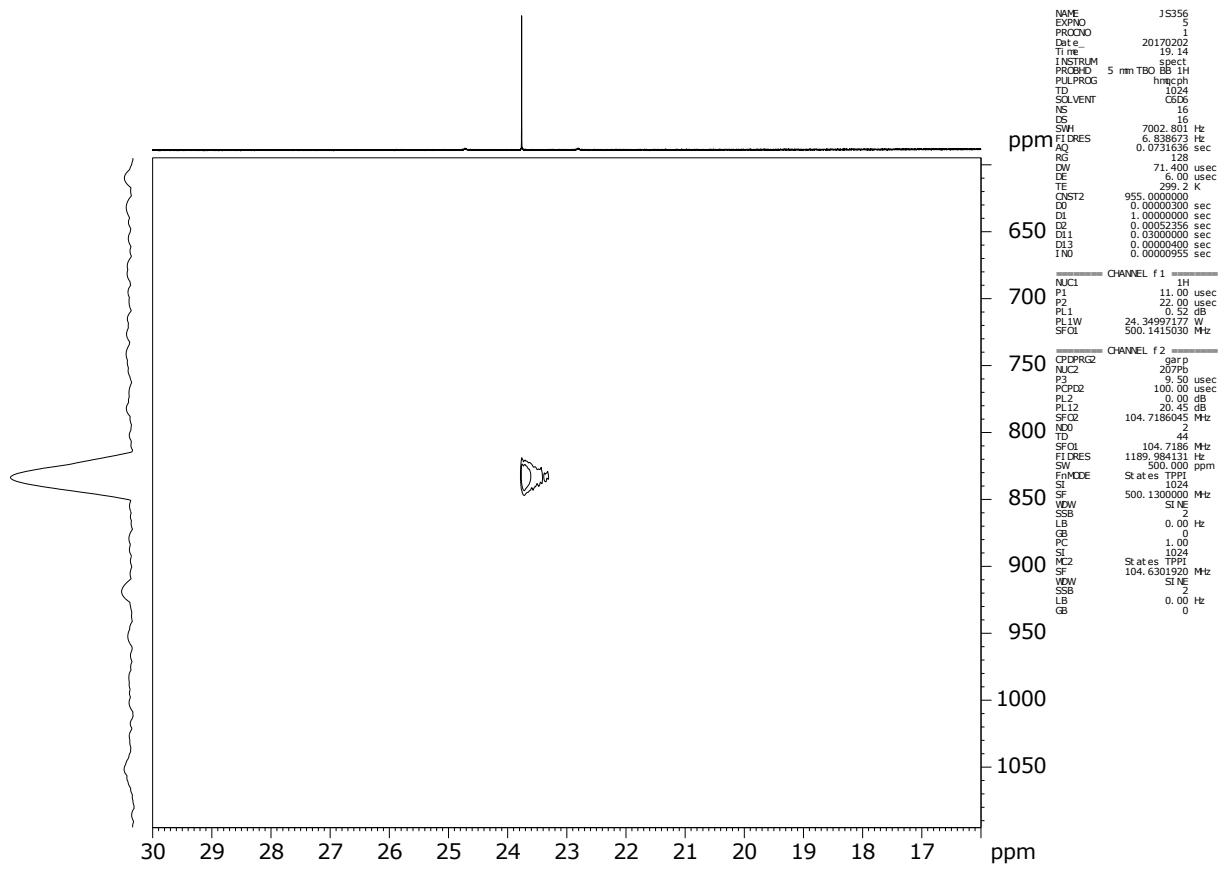


Figure SI7. ^1H - ^{207}Pb HMQC NMR at 26°C of the NHC adduct of Ar*PbH (**5**).

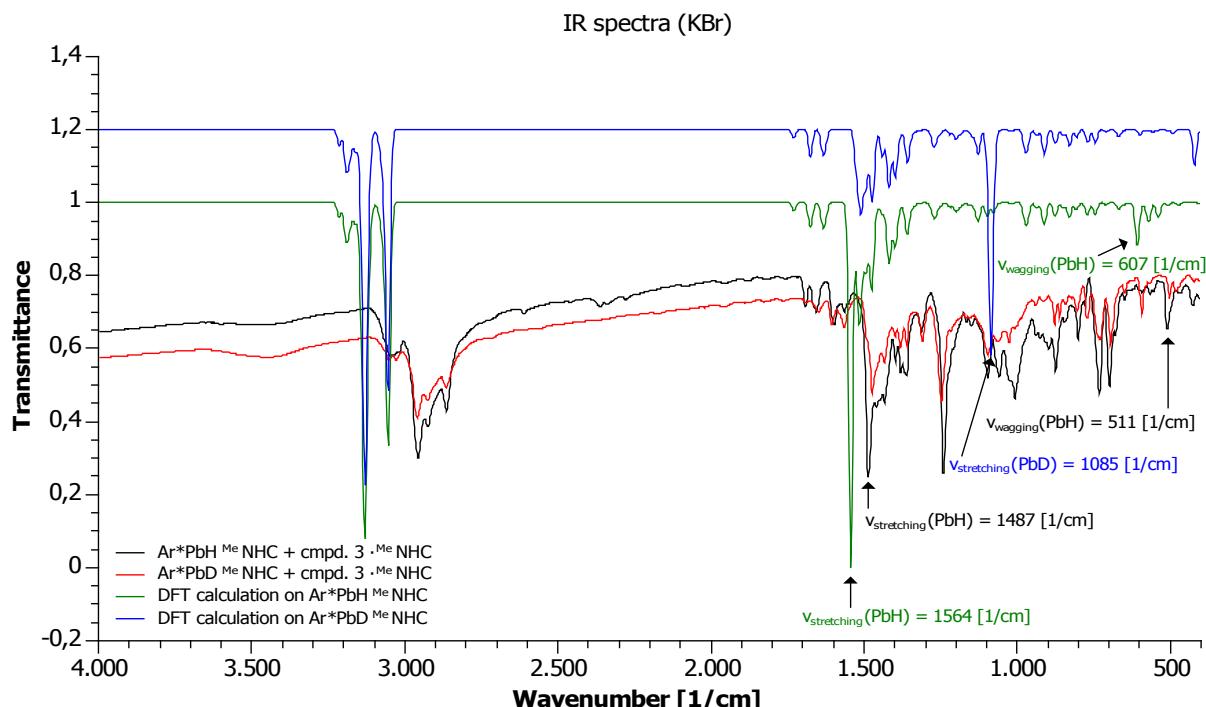


Figure SI8. IR spectra (KBr) of the reaction mixture of lead hydride ^{Me}NHC adduct **5** or deuteride **5-D** and ^{Me}NHC adduct of boryl-phosphinylmethane **3** compared to the results of DFT calculations for the pure hydride/deuteride (for details on DFT calculations see chapter 7).

N. B. The deuteride compound was generated *in situ* along the lines of the hydride **2** procedure using an *in situ* prepared solution of catB-D in thf without further purification.² The IR was taken of the reaction mixture to which ^{Me}NHC was added after removal of all volatiles.

The IR spectrum of the crude reaction mixture of lead hydride ^{Me}NHC adduct **5** and the ^{Me}NHC adduct of boryl-phosphinylmethane **3** shows a PbH stretching band at 1487 cm⁻¹ and a PbH wagging band at 511 cm⁻¹ which are both not observable in the spectrum of the respective deuteride reaction mixture. The PbD stretching band is expected, according to the DFT calculation, at ca. 1000 cm⁻¹, unfortunately overlapped by ^{Me}NHC bands.

5. Subsequent reaction of the [Ar*PbH]₂ (**2**) at 10 °C

By dissolving crystals of [Ar*PbH]₂ (**2**) in organic solvents like toluene or benzene and storing the solution at temperatures above -40 °C a subsequent reaction is observed. The ¹H-NMR spectrum reveals the formation of H₂ and the alkyne analogue [Ar*Pb]₂ (**4**) (see Figure SI9). At ambient temperature the hydride (c = 10.3 mg/mL) is completely decomposed after 2.5 hours. At 10 °C half-life t_{0.5} is determined to be ca. 7.6 hours. During the formation of [Ar*Pb]₂ (**4**) small amounts of elemental lead are formed as well.

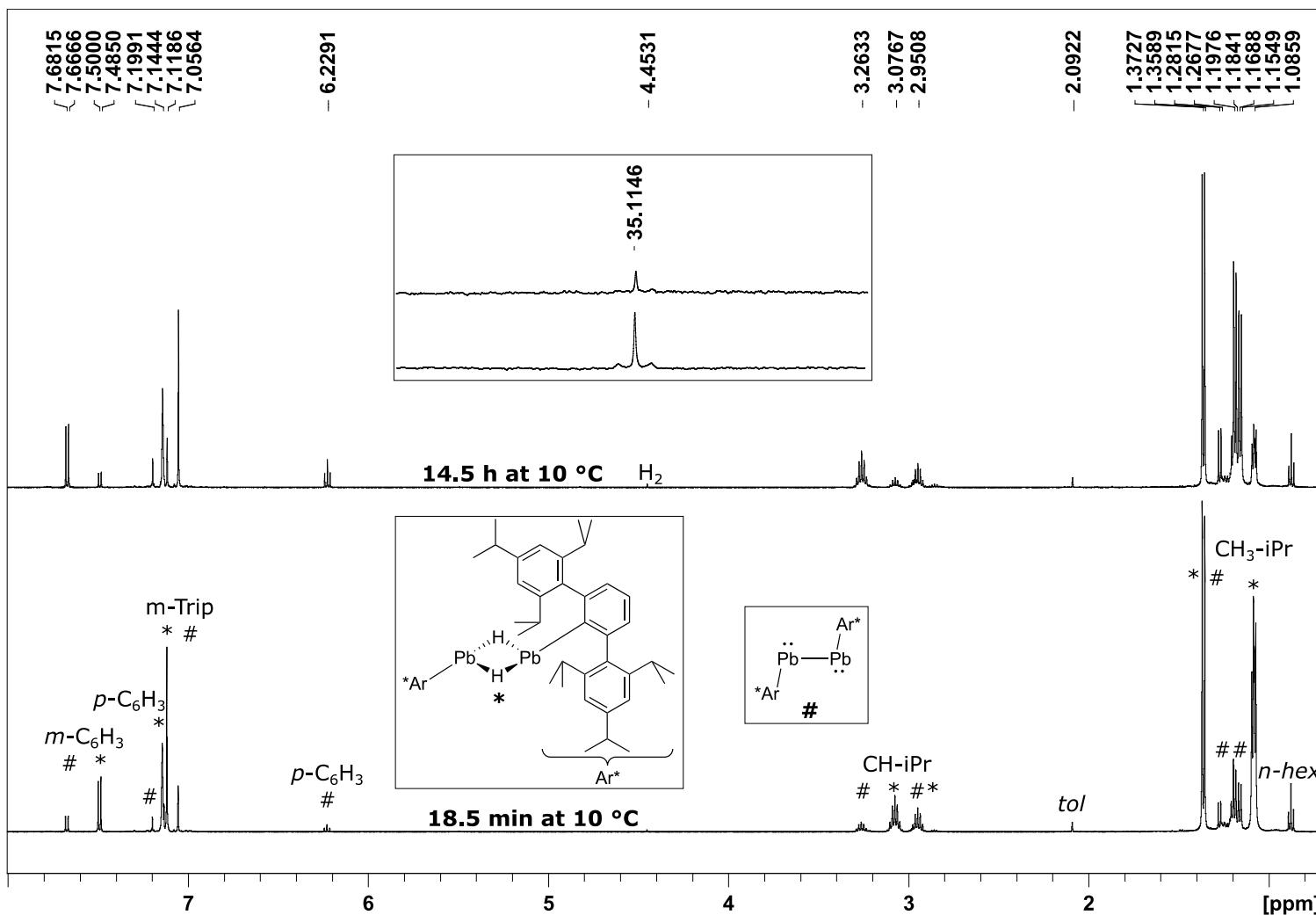


Figure SI9. ^1H NMR spectra of a crystalline lead hydride sample at 10 °C forming the alkyne analogue $[\text{Ar}^*\text{Pb}]_2$. ^1H NMR spectra (500.13 MHz, C_6D_6)

6. Crystal structure analysis of $[\text{Ar}^*\text{PbH}]_2$ (2) and $[\text{Ar}^*\text{PbH}(\text{MeNHC})]$ (5)

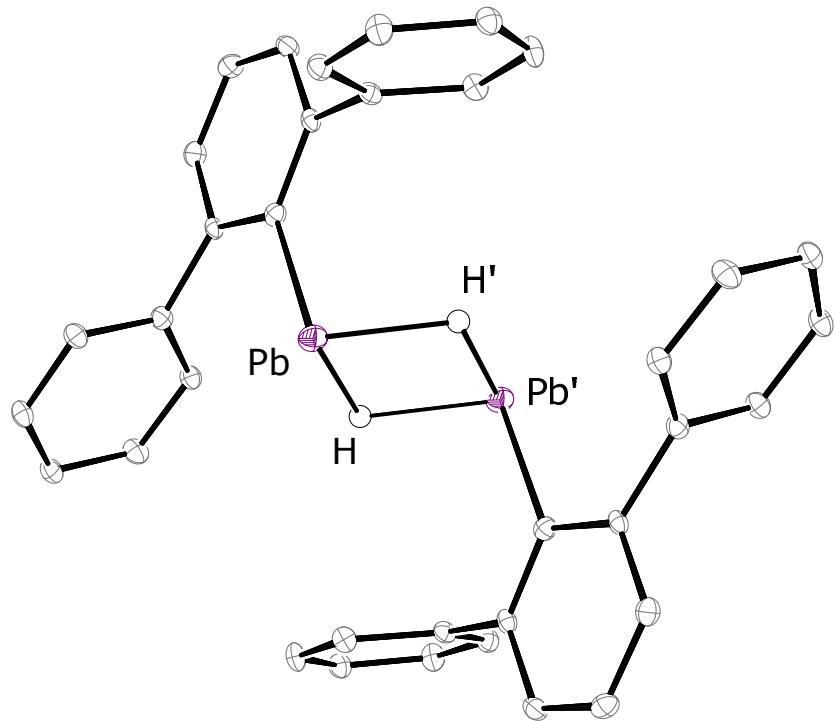


Figure SI10. ORTEP of the molecular structure of $[\text{Ar}^*\text{PbH}]_2$ **2** [$\text{Ar}^* = \text{C}_6\text{H}_3\text{-}2,6\text{-}(\text{C}_6\text{H}_2\text{-}2,4,6\text{-iPr}_3)_2$]. Thermal ellipsoids are shown at 50% probability level. Cocrystallized n-hexane, isopropyl groups and hydrogen atoms except hydrides have been omitted for clarity. Atoms H (and H') were found and refined isotropically in these positions. Selected bond lengths [\AA] and angle [$^\circ$]: Pb-Pb' 3.2646(2), Pb-C 2.306(2), Pb-H 1.98(4), Pb'-H 2.03(4), C1-Pb-Pb' 92.4(1).

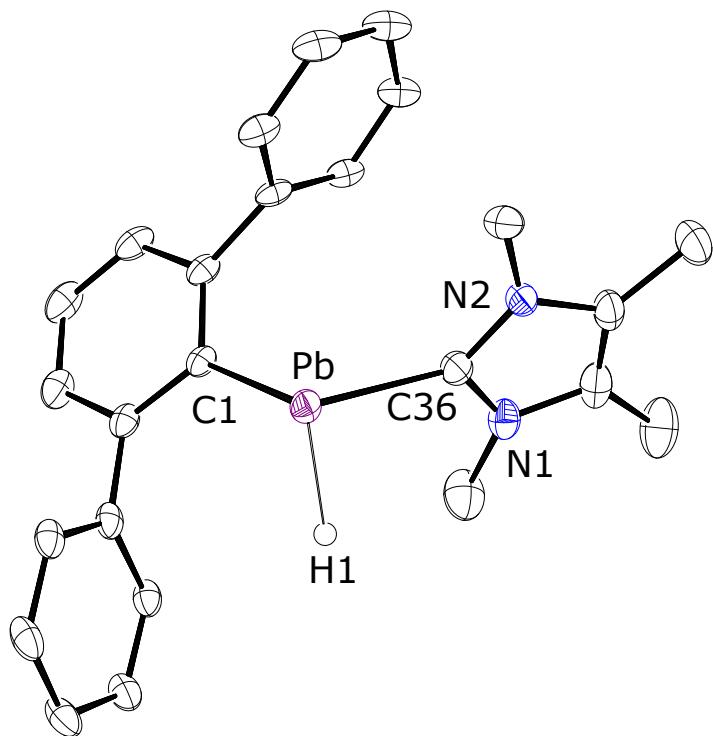


Figure SI11. ORTEP of the molecular structure of $[\text{Ar}^*\text{PbH}(\text{MeNHC})] \mathbf{5}$ [$\text{Ar}^* = \text{C}_6\text{H}_3\text{-2,6-(C}_6\text{H}_2\text{-2,4,6-iPr}_3)_2$]. Thermal ellipsoids are shown at 50% probability level. Isopropyl groups and hydrogen atoms except the hydride H1 have been omitted for clarity. The Pb-hydride moiety is disordered over two positions with a ratio of 4:1. Distances were listed for the main component of the structure. Atom H1 was found and refined with fixed distance. Selected bond lengths [Å] and angle [°]: Pb–C1 2.332(2), Pb–C36 2.411(2), Pb–H1 1.86(2), C1–Pb–C36 98.7(1), C1–Pb–H1 95.1(1), C36–Pb–H1 85.5(1).

Refinement details

X-ray data for **2** and **5** were collected with a Bruker Smart APEX II diffractometer with graphite-monochromated Mo K α radiation. The programs used were Bruker's APEX2 v2011.8-0 including SADABS for absorption correction and SAINT for structure solution, as well as the ShelXLE graphical user interface for shelxl for structure refinement.⁵⁻⁹ For further refinement details see the cif-file.

Results of the crystal structure analysis of 2 and 5.

	[Ar*PbH] ₂ (2)·C ₆ H ₁₄	Ar*PbH ^{Me} NHC (5)
Empirical formula	C ₇₈ H ₁₁₄ Pb ₂	C ₄₃ H ₆₂ N ₂ Pb
M _r / g mol ⁻¹	1466.09	814.13
λ / Å	0.71073	0.71073
T / K	100(2)	100(2)
Crystal system	monoclinic	triclinic
Space group	P2 ₁ /c	P-1
Z	2	2
a / Å	13.2953(3)	12.2209(3)
b / Å	15.9523(4)	12.6206(3)
c / Å	16.9850(4)	14.2456(4)
α	90	75.9180(10)
β	104.3560(10)	77.4530(10)
γ	90	75.3800(10)
V / Å ³	3489.87(14)	2033.52(9)
D _c / g cm ⁻³	1.395	1.330
μ / mm ⁻¹	4.858	4.177
F(000)	1492	832
Crystal size / mm	0.1 x 0.1 x 0.1	0.22 x 0.14 x 0.13
Θ range / °	1.60 - 26.02	2.48 - 27.88
Limiting indices	-19 ≤ h ≤ 19 -23 ≤ k ≤ 23 -24 ≤ l ≤ 24	-16 ≤ h ≤ 15 -16 ≤ k ≤ 16 -18 ≤ l ≤ 18
Reflects. collect.	67957	46452
Indepdnt Reflects	11431	9621
R _{int}	0.0429	0.0265
Completeness	98.3	99.1
Absorp. Corr.	numerical	numerical
Trans. (max., min.)	1.0000, 0.8201	1.0000, 0.7545
Parameters/restraints	365/0	449/2
R ₁ , ωR ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.0282, 0.0572	0.0213, 0.0468
R ₁ , ωR ₂ (all data)	0.0444, 0.0616	0.0247, 0.0476
GooF on F ²	1.018	1.105
Δρ _{max,min} / e·Å ⁻³	3.601, -1.330	0.690, -0.668
CCDC	1531247	1541061

7. Computational Details: structure optimisation, frequency calculation and thermochemical approximations

All structures have been structurally optimised using Gaussian (Version G09.D01)¹⁰ using M06-2X functional¹¹ which has been recommended for main-group thermodynamics and non-covalent interactions with 6-31G(d,p) basis set¹² on light elements and def2TZVP¹³⁻¹⁴ basis set for Pb including Stuttgart-Dresden ECP¹⁵. Frequency calculations revealed no imaginary frequencies. Input structures were taken where obtainable from the experimentally observed X-ray diffraction structures.¹⁶

A summary of the computed energies is listed in Table A:

entry	compound	E(abs) (a.u. -->)	E(ZPVE)	H	G	dE(kcal/mol) -->	dE(ZPVE)	dH	dG
1	RPbH-Dimer	-3188,941445	-3187,404836	-3187,319827	-3187,525352				
2	RPb-PbR	-3187,757861	-3186,234463	-3186,149558	-3186,356356				
3	Hydrogen	-1,168402	-1,158212	-1,154907	-1,169693				
4	PbH-Monomer	-1594,436967	-1593,670187	-1593,627108	-1593,746767				
RXN 1		1 --> 4 + 4				42,36	40,45	41,17	19,97
RXN 2		1 --> 2+3				9,53	7,63	9,64	-0,44

In order to screen for possible isomerism of Ar*Pb(μ-H)₂Ar* and decomposition pathways some isomers have been probed by means of a DFT study with lower level of theory (M06-2X / 6-31G* (C,H) and def2svp+ECP (Pb)). Isomers taken into consideration were based on species already suggested by *Vicha* and *Straka* et al.¹⁷ and Ar* derivatives of species that were discussed in an extensive computational study of related digermynes and distannynes by *Wang* and *Schleyer* et al.¹⁸ All computations revealed no imaginary frequencies or one strong imaginary frequency (i1397 cm⁻¹) for the transition state.

All isomers probed computationally are higher in energy and are unlikely to cause the second ¹H NMR signal observed in solution at low temperatures. Moreover the lower symmetry of these species in terms of their Pb₂H₂ core moiety does not coincide with the symmetry indicated by the isotopomeric distribution of this ¹H-NMR signal. We consider rotations around the Pb-C bonds enclosing the preserved Pb(μ-H)₂Pb moiety to generate the species responsible for the observed second signal set.

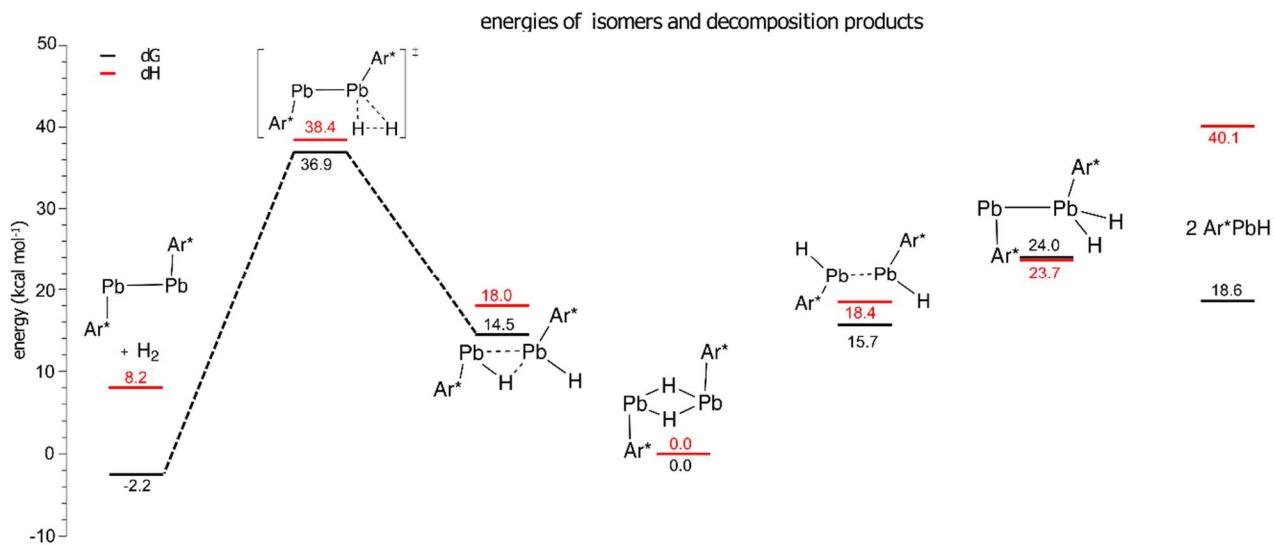


Figure SI12 gives a comparison of the relative energy levels of various isomers and decomposition products.

A summary of the computed energies (M06-2X / 6-31G* (C,H) def2svp+ECP (Pb)) is listed in Table B:

entry	compound	E(abs) (a.u)	E(ZPVE)	H	G	dE(kcal/mol)	dE(ZPVE)	dH	dG
1b	H_2	-1,163713	-1,153392	-1,150087	-1,164864				
2b	PbH Monomer	-1594,055812	-1593,282885	-1593,239888	-1593,359577				
3b	RPbPbR	-3187,000585	-3185,465312	-3185,380611	-3185,587330				
1b+3b	RPbPbR+ H_2	-3188,164298	-3186,618704	-3186,530698	-3186,752194				
4b	TS	-3188,114426	-3186,567785	-3186,482473	-3186,689955				
5b	RHPb(μH)PbR	-3188,147721	-3186,600920	-3186,514975	-3186,725640				
6b	RH ₂ PbPbR	-3188,140597	-3186,590824	-3186,505934	-3186,710438				
7b	RHPb-PbHR	-3188,147526	-3186,600015	-3186,514253	-3186,723804				
8b	RPb(μH) ₂ PbR	-3188,176943	-3186,628454	-3186,543693	-3186,748759				
RXN 1	8b \rightarrow 1b+3b					7,93	6,12	8,15	-2,16
RXN 2	8b \rightarrow 2b + 2b					40,99	39,33	40,11	18,58
RXN 6	8b \rightarrow 5b					18,34	17,28	18,02	14,51
RXN 7	8b \rightarrow 6b					22,81	23,61	23,69	24,05
RXN 8	8b \rightarrow 4b					39,23	38,07	38,42	36,90
RXN 9	8b \rightarrow 7b					18,46	17,85	18,47	15,66

The energy gap between Ar*Pb(μ -H)₂Ar* (entry 8b) and isomer Ar*HPb(μ -H)₁PbAr* (entry 5b) is large. From Ar*HPb(μ -H)₁PbAr* a transition state leading to dehydrogenation and formation of the diplumbyne was found, however with a high activation energy barrier. A very similar hydrogenation route was discussed for the formation of tin(II) hydrides from distannynes.¹⁸ The overall barrier between Ar*Pb(μ -H)₂Ar* and the dehydrogenation transition state is very high to render this pathway unlikely for the diplumbyne formation.

8. Exemplary input file for small basis set calculations

```
%NProcShared=8

%mem=32000mb
%chk=name.chk
# M062X/gen opt(tight,calcfc) freq integral=ultrafinegrid pseudo=read gfinput

//description//


0 1
input structure

H C 0
6-31G*
*****
Pb      0
def2svp
*****


PB      0
PB-ECP   3     60
f-ul potential
 2
2      3.88751200      12.20989200
2      3.81196300      16.19029100
s-ul potential
 4
2      12.29630300     281.28549900
2      8.63263400      62.52021700
2      3.88751200     -12.20989200
2      3.81196300     -16.19029100
p-ul potential
 6
2      10.24179000     72.27689700
2      8.92417600     144.59108300
2      6.58134200      4.75869300
2      6.25540300      9.94062100
2      3.88751200     -12.20989200
2      3.81196300     -16.19029100
d-ul potential
 6
2      7.75433600      35.84850700
2      7.72028100      53.72434200
2      4.97026400      10.11525600
2      4.56378900      14.83373100
2      3.88751200     -12.20989200
2      3.81196300     -16.19029100
```

9. Exemplary input file for larger basis set calculations

```
%NProcShared=8

%mem=32000mb
%chk=name.chk
# M062X/gen opt(tight,calcfc) freq integral=ultrafinegrid pseudo=read gfinput
//description//

0 1
Input structure

H C 0
6-311G(d,p)
*****
Pb      0
S     4   1.00
      591.61124370      0.22126521076E-03
      46.757232559      0.56961959130E-02
      20.746462696      -0.21374063831
      14.610796419      0.40502620616
S     2   1.00
      20.222637612      -0.83541883299E-01
      6.4767324865      0.97910892388
S     1   1.00
      1.6600600927      1.0000000
S     1   1.00
      0.80431655001      1.0000000
S     1   1.00
      0.22627039020      1.0000000
S     1   1.00
      0.84014530665E-01      1.0000000
P     3   1.00
      15.189102118      0.61952303583
      14.693144415      -0.72498497086
      6.8705890048      0.37680007984
P     3   1.00
      2.2021426123      0.40196284806
      1.2209125119      0.46058131862
      0.63367559815      0.19367655397
P     1   1.00
      0.28202837058      1.0000000
P     1   1.00
      0.11333375666      1.0000000
P     1   1.00
      0.43948707430E-01      1.0000000
D     6   1.00
      61.315369628      0.33870800787E-03
      12.372195840      0.13788683942E-01
      6.9254944983      -0.75979608103E-01
      2.3319539939      0.28113784298
      1.2108730003      0.44474512269
      0.60090478506      0.35326874351
D     1   1.00
      0.28135869813      1.0000000
D     1   1.00
      0.115000000000      1.0000000
F     1   1.00
      0.2896200      1.0000000
F     1   1.00
      1.0000000      1.0000000
*****
PB      0
PB-ECP    3       60
```

```

f-ul potential
 2
2      3.88751200          12.20989200
2      3.81196300          16.19029100
s-ul potential
 4
2      12.29630300         281.28549900
2      8.63263400          62.52021700
2      3.88751200          -12.20989200
2      3.81196300          -16.19029100
p-ul potential
 6
2      10.24179000         72.27689700
2      8.92417600          144.59108300
2      6.58134200          4.75869300
2      6.25540300          9.94062100
2      3.88751200          -12.20989200
2      3.81196300          -16.19029100
d-ul potential
 6
2      7.75433600          35.84850700
2      7.72028100          53.72434200
2      4.97026400          10.11525600
2      4.56378900          14.83373100
2      3.88751200          -12.20989200
2      3.81196300          -16.19029100

```

10. Optimized structures for small basis sets

Entry 2b // Ar*PbH monomer

Pb	0.093536000	-0.288576000	-1.166706000
C	-0.045015000	0.786178000	3.810944000
H	-0.065681000	1.033178000	4.868026000
C	0.005635000	0.153336000	1.096221000
C	1.202032000	0.241371000	1.815613000
C	-1.238893000	0.714545000	3.092927000
H	-2.186637000	0.917950000	3.586489000
C	-1.214210000	0.393422000	1.732454000
C	-2.441378000	0.332402000	0.873473000
C	-3.066658000	-0.911582000	0.618541000
C	-4.151474000	-0.951494000	-0.255379000
H	-4.633822000	-1.904981000	-0.454602000
C	-4.636365000	0.197289000	-0.886620000
C	-5.815946000	0.120790000	-1.836959000
H	-6.019001000	1.140452000	-2.188660000
C	-7.074450000	-0.394063000	-1.129738000
H	-6.930210000	-1.421144000	-0.777191000
H	-7.322304000	0.226676000	-0.263976000
H	-7.929084000	-0.392680000	-1.814078000
C	-5.487133000	-0.744000000	-3.059343000
H	-4.602440000	-0.368169000	-3.581710000
H	-5.286559000	-1.778534000	-2.759879000
H	-6.326221000	-0.754862000	-3.762626000
C	-3.999152000	1.406222000	-0.631894000
H	-4.365352000	2.305810000	-1.123365000
C	-2.900511000	1.497045000	0.229817000
C	-2.250504000	2.852662000	0.463382000
H	-1.349999000	2.698552000	1.066105000
C	-3.189193000	3.767847000	1.259112000
H	-4.115560000	3.953500000	0.704006000
H	-3.457046000	3.314058000	2.218166000
H	-2.712006000	4.733660000	1.455162000
C	-1.820825000	3.519878000	-0.847844000
H	-1.154125000	2.870504000	-1.426612000
H	-2.683496000	3.762018000	-1.477836000
H	-1.287279000	4.453555000	-0.640734000
C	-2.602570000	-2.169649000	1.337453000
H	-1.523722000	-2.073280000	1.504879000
C	-3.287786000	-2.267133000	2.707943000
H	-3.066473000	-1.392664000	3.326264000
H	-4.374783000	-2.331691000	2.583828000
H	-2.950385000	-3.160418000	3.244153000
C	-2.830672000	-3.453995000	0.538601000
H	-3.895095000	-3.704457000	0.467418000
H	-2.421707000	-3.371126000	-0.472664000
H	-2.334392000	-4.291194000	1.039257000
C	2.450059000	0.009247000	1.016992000
C	2.767458000	-1.303936000	0.596604000
C	3.811420000	-1.483156000	-0.318383000
H	4.060830000	-2.486012000	-0.654017000
C	4.556289000	-0.412401000	-0.806358000
C	5.674535000	-0.633633000	-1.806801000
H	5.724844000	-1.711466000	-2.007142000
C	5.384303000	0.079897000	-3.132206000

H	4.426091000	-0.240557000	-3.551732000
H	5.342426000	1.165103000	-2.988075000
H	6.170653000	-0.130483000	-3.864336000
C	7.028795000	-0.195081000	-1.238349000
H	7.035395000	0.881585000	-1.035895000
H	7.250422000	-0.714380000	-0.301610000
H	7.832747000	-0.406294000	-1.950859000
C	4.250350000	0.869006000	-0.347332000
H	4.833221000	1.710445000	-0.713174000
C	3.210731000	1.104321000	0.552724000
C	2.870850000	2.528464000	0.974051000
H	2.452713000	2.484517000	1.984797000
C	4.088792000	3.455088000	1.018027000
H	4.912776000	3.012015000	1.585676000
H	3.814818000	4.402641000	1.491652000
H	4.454746000	3.691169000	0.013021000
C	1.790421000	3.117243000	0.055583000
H	0.865684000	2.534334000	0.111160000
H	1.558548000	4.148756000	0.343524000
H	2.133466000	3.120385000	-0.985832000
C	2.074639000	-2.507363000	1.225568000
H	1.019733000	-2.252653000	1.372529000
C	2.128872000	-3.775740000	0.373649000
H	1.772061000	-3.593801000	-0.644576000
H	3.143820000	-4.185580000	0.321815000
H	1.490234000	-4.543424000	0.820979000
C	2.689793000	-2.772897000	2.607999000
H	3.757974000	-2.997801000	2.511319000
H	2.580449000	-1.904364000	3.263669000
H	2.201039000	-3.627957000	3.086696000
H	-0.263738000	-2.106386000	-0.874079000
C	1.175676000	0.551667000	3.178537000
H	2.104975000	0.617941000	3.740512000

Entry 3b // Ar*PbPbAr* / Diplumbyne

Pb	-0.126204000	1.336779000	0.907835000
C	0.151466000	2.746419000	-0.931446000
C	-1.038590000	3.251608000	-1.478369000
C	-1.016691000	4.141459000	-2.557332000
C	0.197570000	4.549997000	-3.101106000
C	1.385767000	4.087973000	-2.543265000
C	1.368247000	3.198031000	-1.461741000
C	2.679077000	2.834084000	-0.836256000
C	3.452911000	1.773376000	-1.344245000
C	4.753354000	1.587086000	-0.863580000
C	5.303470000	2.423705000	0.109489000
C	4.484575000	3.409417000	0.659353000
C	3.183274000	3.634547000	0.208461000
C	-2.355988000	2.904940000	-0.851067000
C	-3.153225000	1.862046000	-1.371910000
C	-4.428417000	1.661808000	-0.846623000
C	-4.937501000	2.452533000	0.186578000
C	-4.115731000	3.437521000	0.725291000
C	-2.827991000	3.673436000	0.233973000
C	-1.997820000	4.802255000	0.828122000
C	-2.436212000	6.147664000	0.235730000
C	-2.049681000	4.837349000	2.358500000
C	-6.348197000	2.192875000	0.688038000
C	-7.373235000	2.555984000	-0.395082000
C	-6.685578000	2.903229000	1.997659000
C	-2.656278000	0.995450000	-2.518086000
C	-3.033679000	-0.477266000	-2.338492000
C	-3.185827000	1.515555000	-3.860668000
C	2.917446000	0.891509000	-2.462876000
C	3.475683000	1.340856000	-3.818928000
C	3.210523000	-0.591592000	-2.230020000
C	6.754865000	2.331804000	0.555571000
C	7.712118000	2.013551000	-0.595926000
C	6.953780000	1.335605000	1.703335000
C	2.384586000	4.787982000	0.798039000
C	2.226797000	4.656244000	2.316293000
C	3.018767000	6.132850000	0.423308000
H	-1.954062000	4.527185000	-2.952651000
H	0.218433000	5.243055000	-3.936483000
H	2.341750000	4.435934000	-2.928684000
H	5.363303000	0.799005000	-1.299705000
H	4.897120000	4.057091000	1.432107000
H	-5.045015000	0.856992000	-1.240030000
H	-4.477417000	4.045452000	1.548518000
H	-0.954252000	4.637767000	0.540846000
H	-1.830508000	6.964377000	0.642690000
H	-3.486777000	6.348154000	0.475557000
H	-2.328300000	6.148934000	-0.853073000
H	-1.334628000	5.574636000	2.737606000
H	-1.793393000	3.861738000	2.785943000
H	-3.039926000	5.124510000	2.728364000
H	-6.424494000	1.110643000	0.871761000
H	-7.170007000	2.029201000	-1.332495000
H	-7.336615000	3.631483000	-0.600022000
H	-8.387952000	2.301670000	-0.070904000

H	-5.962662000	2.665986000	2.784945000
H	-7.678778000	2.601265000	2.342826000
H	-6.699384000	3.990591000	1.863601000
H	-1.561276000	1.069753000	-2.540354000
H	-2.828283000	-0.831112000	-1.317396000
H	-2.489011000	-1.103990000	-3.053083000
H	-4.101916000	-0.649277000	-2.507629000
H	-2.855626000	2.541319000	-4.045608000
H	-4.282019000	1.502062000	-3.865500000
H	-2.831452000	0.886737000	-4.684229000
H	1.827890000	1.019351000	-2.492048000
H	3.205942000	2.379503000	-4.030337000
H	3.083594000	0.712659000	-4.625715000
H	4.569162000	1.264118000	-3.825564000
H	2.895972000	-0.914055000	-1.227792000
H	4.282313000	-0.809651000	-2.301024000
H	2.699653000	-1.207878000	-2.978228000
H	7.019864000	3.326039000	0.938439000
H	7.569667000	2.701570000	-1.434211000
H	7.565193000	0.993061000	-0.967438000
H	8.750178000	2.089364000	-0.257079000
H	6.262445000	1.531837000	2.529395000
H	7.976436000	1.392927000	2.091336000
H	6.791335000	0.310763000	1.353460000
H	1.382176000	4.764780000	0.360638000
H	1.715385000	3.723277000	2.578952000
H	1.634033000	5.488892000	2.710086000
H	3.196817000	4.666699000	2.825732000
H	3.090674000	6.238853000	-0.663543000
H	4.028514000	6.221108000	0.839643000
H	2.418963000	6.962677000	0.811584000
Pb	-0.001434000	-1.311185000	-0.893138000
C	-0.127299000	-2.729271000	0.952474000
C	1.043197000	-3.195714000	1.568015000
C	0.982279000	-4.081291000	2.649306000
C	-0.248700000	-4.534294000	3.115205000
C	-1.415595000	-4.120908000	2.478691000
C	-1.358409000	-3.226926000	1.402551000
C	-2.632498000	-2.880281000	0.694676000
C	-3.500651000	-1.900809000	1.219610000
C	-4.762391000	-1.731770000	0.642532000
C	-5.184145000	-2.508480000	-0.439182000
C	-4.277628000	-3.410662000	-0.992158000
C	-3.003507000	-3.608192000	-0.455637000
C	-2.090031000	-4.666940000	-1.058145000
C	-2.078011000	-4.640712000	-2.589066000
H	-1.846874000	-3.638385000	-2.966062000
H	-1.315740000	-5.329559000	-2.967130000
H	-3.038830000	-4.952425000	-3.012485000
C	-2.473956000	-6.057666000	-0.537216000
H	-2.413380000	-6.095469000	0.554664000
H	-3.499196000	-6.309015000	-0.832491000
H	-1.802937000	-6.821000000	-0.945990000
H	-1.068763000	-4.459621000	-0.722476000
H	-4.590856000	-4.002101000	-1.849770000
C	-6.609938000	-2.450302000	-0.959683000
C	-7.581829000	-2.974950000	0.105373000
H	-7.303825000	-3.982069000	0.428719000
H	-7.572540000	-2.324395000	0.987165000
H	-8.605272000	-3.003558000	-0.282939000
C	-7.035303000	-1.055557000	-1.423602000
H	-6.386391000	-0.679671000	-2.221572000
H	-8.062092000	-1.074351000	-1.803925000
H	-7.004791000	-0.341597000	-0.593487000
H	-6.664864000	-3.122533000	-1.825422000
H	-5.446197000	-1.001648000	1.073856000
C	-3.097377000	-1.079253000	2.435662000
C	-3.771231000	-1.615611000	3.704726000
H	-3.495349000	-2.657439000	3.889782000
H	-3.477343000	-1.022561000	4.577129000
H	-4.862004000	-1.564286000	3.608535000
C	-3.405080000	0.408556000	2.258437000
H	-3.024815000	0.786745000	1.300881000
H	-4.484287000	0.602502000	2.267000000
H	-2.958439000	0.994329000	3.069578000
H	-2.012877000	-1.183909000	2.560904000
H	-2.380467000	-4.507041000	2.800380000
H	-0.297038000	-5.227307000	3.949480000
H	1.905439000	-4.436542000	3.102321000
C	2.379798000	-2.845416000	0.991707000
C	3.110455000	-1.734802000	1.462857000
C	4.392840000	-1.513847000	0.966331000
C	4.973141000	-2.348461000	0.008943000
C	4.219555000	-3.411620000	-0.477744000
C	2.928442000	-3.673600000	-0.007983000
C	2.178000000	-4.880171000	-0.553998000
C	2.853909000	-6.181357000	-0.104950000
H	2.294413000	-7.050403000	-0.466590000
H	3.875087000	-6.248366000	-0.496876000
H	2.906688000	-6.235696000	0.986807000
C	2.040216000	-4.829732000	-2.079524000
H	1.458155000	-5.687482000	-2.434073000
H	1.528357000	-3.914731000	-2.399745000
H	3.016661000	-4.863508000	-2.575506000
H	1.168417000	-4.873205000	-0.132525000
H	4.638845000	-4.062673000	-1.240357000
C	6.394267000	-2.067627000	-0.444792000
C	7.389907000	-2.504698000	0.638891000
H	7.161102000	-2.039040000	1.602444000
H	7.343689000	-3.590965000	0.773868000
H	8.413932000	-2.235146000	0.358749000
C	6.760265000	-2.700885000	-1.786472000

H	6.036252000	-2.446455000	-2.567268000
H	7.747725000	-2.356076000	-2.107989000
H	6.804489000	-3.792770000	-1.708017000
H	6.479687000	-0.976825000	-0.553206000
H	4.958703000	-0.657849000	1.324506000
C	2.542261000	-0.818328000	2.533785000
C	2.893154000	0.652063000	2.288257000
H	2.694380000	0.952759000	1.247753000
H	2.330532000	1.299969000	2.969231000
H	3.956131000	0.854955000	2.457654000
C	3.022007000	-1.255304000	3.923738000
H	2.711541000	-2.281328000	4.140796000
H	4.115776000	-1.208932000	3.978494000
H	2.610722000	-0.599923000	4.698678000
H	1.449186000	-0.921595000	2.514196000

Entry 4b // TRANSITION STATE / Diplumbyne + H₂ → Ar*HPb(μ-H)PbAr*

Pb	-0.322737000	-1.369747000	-0.828595000
C	-0.181607000	-2.731244000	1.046665000
C	-1.386939000	-3.152097000	1.629898000
C	-1.386353000	-4.089999000	2.667341000
C	-0.186983000	-4.634409000	3.115674000
C	1.007526000	-4.262946000	2.506081000
C	1.020721000	-3.314839000	1.474283000
C	2.322952000	-3.056418000	0.772165000
C	3.299218000	-2.212424000	1.336224000
C	4.565432000	-2.141856000	0.741529000
C	4.892502000	-2.883331000	-0.390950000
C	3.889808000	-3.665674000	-0.967798000
C	2.611910000	-3.763372000	-0.420349000
C	-2.687062000	-2.744419000	1.000704000
C	-3.440160000	-1.642324000	1.471100000
C	-4.655679000	-1.354854000	0.855545000
C	-5.156160000	-2.115458000	-0.206509000
C	-4.396629000	-3.185726000	-0.661631000
C	-3.167358000	-3.516064000	-0.078163000
C	-2.438668000	-4.760985000	-0.570425000
C	-3.211508000	-6.018965000	-0.152802000
C	-2.197561000	-4.751117000	-2.083376000
C	-6.492639000	-1.731212000	-0.818344000
C	-7.628353000	-1.960702000	0.187925000
C	-6.799198000	-2.437564000	-2.137500000
C	-2.961905000	-0.814637000	2.654578000
C	-3.486623000	-0.623187000	2.631110000
C	-3.363560000	-1.483023000	3.977967000
C	3.026638000	-1.424328000	2.610810000
C	3.479849000	-2.204028000	3.853792000
C	3.698815000	-0.046354000	2.611379000
C	6.285517000	-2.902730000	-1.005613000
C	7.369077000	-2.316569000	-0.102227000
C	6.314582000	-2.207734000	-2.373529000
C	1.593920000	-4.698702000	-1.062761000
C	1.624805000	-4.661636000	-2.593338000
C	1.784449000	-6.132514000	-0.551979000
H	-2.331257000	-4.426846000	3.087145000
H	-0.186145000	-5.375786000	3.908766000
H	1.939387000	-4.738384000	2.802558000
H	5.321074000	-1.515136000	1.206098000
H	4.131332000	-4.242545000	-1.858574000
H	-5.229329000	-0.494366000	1.189876000
H	-4.759595200	-3.791660000	-1.486674000
H	-1.461416000	-4.806570000	-0.081132000
H	-2.674060000	-6.921285000	-0.463060000
H	-4.205300000	-6.038153000	-0.613983000
H	-3.342414000	-6.052096000	0.933085000
H	-1.641084000	-5.647467000	-2.379304000
H	-1.615741000	-3.874584000	-2.393512000
H	-3.137493000	-4.745400000	-2.645735000
H	-6.443420000	-0.651690000	-1.025110000
H	-7.446536000	-1.427273000	1.125849000

H	-7.715619000	-3.027995000	0.419042000
H	-8.584426000	-1.617735000	-0.221502000
H	-5.997933000	-2.292754000	-2.869600000
H	-7.727559000	-2.047636000	-2.565049000
H	-6.932880000	-3.514608000	-1.986094000
H	-1.865228000	-0.781741000	2.611792000
H	-3.379600000	1.085942000	1.645677000
H	-2.936492000	1.233802000	3.354253000
H	-4.546077000	0.659780000	2.912850000
H	-2.913759000	-2.472105000	4.088281000
H	-4.452930000	-1.592013000	4.027992000
H	-3.043145000	-0.866853000	4.824717000
H	1.941690000	-1.275159000	2.679232000
H	2.936148000	-3.144039000	3.966438000
H	3.316727000	-1.606342000	4.756943000
H	4.549845000	-2.431914000	3.785306000
H	3.559716000	0.477147000	1.660778000
H	4.777363000	-0.129819000	2.794777000
H	3.282197000	0.573447000	3.412815000
H	6.529805000	-3.960702000	-1.174821000
H	7.367017000	-2.780583000	0.888695000
H	7.232426000	-1.236190000	0.024815000
H	8.355150000	-2.469414000	-0.551085000
H	5.549972000	-2.606758000	-3.047144000
H	7.292074000	-2.338228000	-2.849384000
H	6.139448000	-1.130859000	-2.262242000
H	0.595008000	-4.375828000	-0.751907000
H	1.541436000	-3.636338000	-2.970568000
H	0.788692000	-5.241437000	-2.996854000
H	2.545476000	-5.097072000	-2.995626000
H	1.690087000	-6.176386000	0.536983000
H	2.777192000	-6.507180000	-0.826435000
H	1.032809000	-6.799186000	-0.989677000
Pb	0.642052000	1.325959000	0.839954000
C	0.178713000	2.837843000	-0.899152000
C	1.332543000	3.305606000	-1.558819000
C	1.257069000	4.203141000	-2.627608000
C	0.019312000	4.676264000	-3.047386000
C	-1.128741000	4.260646000	-2.381481000
C	-1.063608000	3.348591000	-1.316837000
C	-2.372981000	3.059579000	-0.641676000
C	-3.283075000	2.145983000	-1.206259000
C	-4.592201000	2.098086000	-0.718058000
C	-5.019739000	2.929313000	0.319604000
C	-4.075123000	3.756518000	0.922451000
C	-2.755674000	3.830627000	0.470479000
C	-1.787941000	4.788076000	1.149077000
C	-1.756067000	4.587732000	2.667431000
H	-1.540509000	3.542921000	2.915461000
H	-0.980596000	5.218275000	3.116181000
H	-2.710531000	4.857644000	3.132418000
C	-2.116250000	6.240935000	0.786629000
H	-2.078199000	6.388551000	-0.297313000
H	-3.121187000	6.510081000	1.131625000
H	-1.401213000	6.927318000	1.253610000
H	-0.783008000	4.574654000	0.770656000
H	-4.387802000	4.386893000	1.753099000
C	-6.477725000	3.003403000	0.737152000
C	-7.311913000	3.650803000	-0.376195000
H	-6.914395000	4.634306000	-0.642623000
H	-7.296313000	3.027181000	-1.277247000
H	-8.354954000	3.769206000	-0.063888000
C	-7.071246000	1.647495000	1.124794000
H	-6.515836000	1.191071000	1.949746000
H	-8.115275000	1.758886000	1.436427000
H	-7.053745000	0.954450000	0.276366000
H	-6.528996000	3.655458000	1.618541000
H	-5.305373000	1.420234000	-1.185912000
C	-2.870828000	1.255550000	-2.370466000
C	-3.384336000	1.810336000	-3.705041000
H	-2.983582000	2.808592000	-3.899624000
H	-3.092827000	1.156207000	-4.533906000
H	-4.478315000	1.878220000	-3.692084000
C	-3.342568000	-0.189108000	-2.186793000
H	-3.096479000	-0.567763000	-1.185820000
H	-4.430775000	-0.274705000	-2.290809000
H	-2.892495000	-0.843925000	-2.942225000
H	-1.773613000	1.250626000	-2.408572000
H	-2.098092000	4.659949000	-2.670952000
H	-0.050452000	5.382683000	-3.869040000
H	2.172553000	4.550394000	-3.101645000
C	2.675261000	2.897518000	-1.032562000
C	3.255022000	1.669146000	-1.419494000
C	4.453297000	1.275738000	-0.830385000
C	5.098701000	2.059403000	0.132160000
C	4.509302000	3.262444000	0.501715000
C	3.303334000	3.697367000	-0.063295000
C	2.688814000	5.002647000	0.424884000
C	3.671560000	6.172887000	0.305336000
H	3.180794000	7.110004000	0.587020000
H	4.537120000	6.041601000	0.963591000
H	4.039847000	6.271973000	-0.720161000
C	2.179985000	4.864997000	1.865369000
H	1.736518000	5.805967000	2.209817000
H	1.409223000	4.087725000	1.943211000
H	2.994375000	4.600144000	2.549331000
H	1.826286000	5.232148000	-0.207395000
H	4.979825000	3.878196000	1.263291000
C	6.399043000	1.555830000	0.732478000
C	7.535465000	1.653576000	-0.294122000
H	7.288658000	1.115049000	-1.214900000
H	7.717558000	2.701389000	-0.556931000

H	8.462904000	1.234035000	0.110622000
C	6.791972000	2.249688000	2.035031000
H	5.979797000	2.215369000	2.768568000
H	7.669461000	1.762504000	2.470704000
H	7.051967000	3.299899000	1.861359000
H	6.243003000	0.491189000	0.957753000
H	4.888017000	0.311009000	-1.087161000
C	2.583111000	0.802478000	-2.472439000
C	2.824440000	-0.691831000	-2.260556000
H	2.651506000	-0.992075000	-1.216516000
H	2.172493000	-1.278470000	-2.917725000
H	3.853809000	-0.976499000	-2.497878000
C	3.041804000	1.224130000	-3.874753000
H	2.803453000	2.274057000	-4.067213000
H	4.125944000	1.094193000	-3.970902000
H	2.552504000	0.613926000	-4.641268000
H	1.502019000	0.985610000	-2.412896000
H	-1.232387000	1.211937000	1.356237000
H	-1.137845000	0.280066000	0.453650000

Entry 5b // Ar*HPb(μ-H)PbAr*

C	-0.301616000	-2.728960000	0.997773000
C	0.892707000	-3.254920000	1.514937000
C	-1.527347000	-3.142548000	1.542203000
C	0.847796000	-4.171410000	2.573648000
C	-1.557740000	-4.054394000	2.602743000
C	-0.370495000	-4.564513000	3.119637000
H	1.776070000	-4.593680000	2.951313000
H	-2.515199000	-4.378070000	3.004147000
H	-0.394764000	-5.282351000	3.933882000
C	0.272773000	2.877237000	-0.865641000
C	1.495331000	3.345711000	-1.376809000
C	-0.918202000	3.486818000	-1.291405000
C	1.527669000	4.384611000	-2.313592000
C	-0.870003000	4.532894000	-2.223360000
C	0.343295000	4.973643000	-2.742397000
H	2.486785000	4.741835000	-2.682230000
H	-1.798640000	5.008934000	-2.530150000
H	0.365355000	5.785178000	-3.463410000
C	2.799575000	2.808391000	-0.859115000
C	3.370979000	1.639105000	-1.404328000
C	3.467990000	3.499912000	0.172639000
C	4.623267000	1.223125000	-0.948090000
C	4.723531000	3.050223000	0.589487000
C	5.330782000	1.931337000	0.022722000
H	5.072610000	0.325287000	-1.365905000
H	5.246017000	3.601851000	1.368997000
C	-2.258964000	3.137297000	-0.715459000
C	-2.729695000	3.868109000	0.388334000
C	-3.075156000	2.145227000	-1.302089000
C	-4.038751000	3.659598000	0.838128000
C	-4.358121000	1.946794000	-0.796726000
C	-4.872521000	2.714215000	0.252972000
H	-4.399378000	4.248611000	1.676280000
H	-4.986512000	1.167372000	-1.224804000
C	2.231117000	-2.938662000	0.908881000
C	2.694222000	-3.711623000	-0.176639000
C	3.059683000	-1.937376000	1.457285000
C	3.999819000	-3.527201000	-0.638498000
C	4.349259000	-1.774778000	0.946320000
C	4.852477000	-2.580915000	-0.073829000
H	4.366282000	-4.160267000	-1.444424000
H	4.994458000	-1.006494000	1.367356000
C	-2.820120000	-2.665202000	0.947210000
C	-3.468409000	-1.528286000	1.472564000
C	-3.397049000	-3.370068000	-0.129603000
C	-4.716558000	-1.173084000	0.961846000
C	-4.650270000	-2.974634000	-0.608124000
C	-5.338158000	-1.895579000	-0.057221000
H	-5.231434000	-0.311739000	1.379171000
H	-5.110451000	-3.544783000	-1.412959000
C	2.856380000	4.715579000	0.854479000
H	1.939186000	4.981862000	0.321602000
C	2.672567000	0.871354000	-2.516226000
H	1.592933000	1.042541000	-2.413636000
C	-2.584385000	1.331092000	-2.490800000
H	-1.496960000	1.215934000	-2.383699000

C	-1.864332000	4.904011000	1.091984000
H	-0.833539000	4.774793000	0.745942000
C	-2.726414000	-4.597509000	-0.731926000
H	-1.693872000	-4.634949000	-0.367709000
C	-2.849705000	-0.723237000	2.605374000
H	-1.761618000	-0.859455000	2.550127000
C	2.601428000	-1.079469000	2.627713000
H	1.506328000	-1.021972000	2.585099000
C	1.833861000	-4.794868000	-0.812617000
H	0.806177000	-4.666195000	-0.456809000
C	-2.843066000	2.076650000	-3.808381000
H	-2.505447000	1.476866000	-4.660717000
H	-3.916044000	2.265512000	-3.926620000
H	-2.320168000	3.035333000	-3.837007000
C	-3.212047000	-0.064804000	-2.566992000
H	-4.238010000	-0.014486000	-2.947201000
H	-2.648050000	-0.693995000	-3.265732000
H	-3.249487000	-0.557029000	-1.587497000
C	3.092202000	1.422794000	-3.885530000
H	4.173466000	1.309047000	-4.023477000
H	2.584489000	0.881865000	-4.691130000
H	2.844533000	2.484510000	-3.974673000
C	2.918826000	-0.638191000	-2.444603000
H	2.772156000	-1.026788000	-1.428902000
H	2.238748000	-1.161872000	-3.126121000
H	3.938270000	-0.899424000	-2.748284000
C	1.808664000	-4.695754000	-2.341811000
H	2.789126000	-4.913624000	-2.778298000
H	1.096297000	-5.416820000	-2.756222000
H	1.514156000	-3.693122000	-2.672730000
C	2.301643000	-6.183670000	-0.361073000
H	3.337161000	-6.361905000	-0.672544000
H	2.255117000	-6.273470000	0.728502000
H	1.673801000	-6.966666000	-0.799254000
C	2.977511000	-1.732498000	3.965946000
H	2.497504000	-2.706182000	4.087611000
H	4.062833000	-1.873297000	4.023925000
H	2.670556000	-1.093423000	4.800717000
C	3.167596000	0.347347000	2.585824000
H	2.579755000	1.006356000	3.234448000
H	4.200362000	0.376704000	2.951004000
H	3.180770000	0.765666000	1.571792000
C	-2.676279000	-4.547594000	-2.262850000
H	-2.095798000	-5.391092000	-2.650565000
H	-3.677093000	-4.605579000	-2.703315000
H	-2.212421000	-3.620914000	-2.622546000
C	-3.424875000	-5.875535000	-0.251655000
H	-4.473443000	-5.884105000	-0.569989000
H	-2.935204000	-6.764473000	-0.662978000
H	-3.402035000	-5.942732000	0.840190000
C	-3.325235000	-1.256312000	3.964013000
H	-3.059022000	-2.308114000	4.099807000
H	-2.874731000	-0.680619000	4.779308000
H	-4.414690000	-1.166311000	4.044142000
C	-3.134314000	0.776152000	2.495498000
H	-4.191270000	1.004153000	2.681621000
H	-2.546895000	1.321654000	3.241622000
H	-2.875114000	1.163671000	1.505324000
C	-2.310622000	6.323467000	0.721984000
H	-2.248901000	6.485217000	-0.358658000
H	-3.348255000	6.494600000	1.031131000
H	-1.680964000	7.069719000	1.218257000
C	-1.856779000	4.710781000	2.612212000
H	-1.146578000	5.404406000	3.075111000
H	-2.840831000	4.905487000	3.052514000
H	-1.560380000	3.689718000	2.872272000
C	3.787720000	5.931460000	0.800244000
H	3.292659000	6.807064000	1.232148000
H	4.709204000	5.759557000	1.366925000
H	4.065345000	6.167380000	-0.231650000
C	2.468928000	4.381590000	2.300464000
H	3.344259000	4.063972000	2.879145000
H	2.033223000	5.256864000	2.794432000
H	1.728954000	3.573351000	2.334342000
H	-1.399625000	-0.013497000	-0.067646000
H	-0.128234000	1.805056000	2.108551000
Pb	-0.370541000	-1.492968000	-0.950110000
Pb	0.480890000	1.060401000	0.543781000
C	-6.304769000	2.481343000	0.705311000
H	-6.423077000	1.397875000	0.849527000
C	-6.659727000	3.164955000	2.024303000
H	-6.638652000	4.255534000	1.919353000
H	-7.670526000	2.883050000	2.333943000
H	-5.966070000	2.887020000	2.824325000
C	-7.288248000	2.905358000	-0.394493000
H	-7.089319000	2.378825000	-1.332906000
H	-8.320554000	2.695333000	-0.094861000
H	-7.197807000	3.980086000	-0.586521000
C	-6.750300000	-1.553068000	-0.497390000
H	-7.038272000	-0.627302000	0.018663000
C	-6.868849000	-1.304097000	-2.003233000
H	-7.906373000	-1.080146000	-2.272053000
H	-6.247009000	-0.461576000	-2.318204000
H	-6.557788000	-2.183923000	-2.576969000
C	-7.721250000	-2.657021000	-0.057879000
H	-7.659128000	-2.828729000	1.020522000
H	-8.752917000	-2.390018000	-0.309438000
H	-7.482974000	-3.600117000	-0.562560000
C	6.749054000	1.533840000	0.387925000
H	6.961926000	0.585998000	-0.124624000
C	6.951060000	1.318140000	1.890177000
H	7.990161000	1.044038000	2.099934000

H	6.727995000	2.230497000	2.453823000
H	6.306458000	0.522269000	2.274309000
C	7.739212000	2.581696000	-0.138328000
H	8.771529000	2.275310000	0.060222000
H	7.620320000	2.727968000	-1.215700000
H	7.571550000	3.547022000	0.352248000
C	6.310788000	-2.485692000	-0.483991000
H	6.734770000	-1.611669000	0.028587000
C	7.070780000	-3.726631000	0.004567000
H	6.688660000	-4.627668000	-0.488341000
H	8.138773000	-3.643263000	-0.222182000
H	6.952919000	-3.859190000	1.083817000
C	6.513239000	-2.298663000	-1.990066000
H	6.078079000	-3.130685000	-2.554187000
H	6.053489000	-1.373709000	-2.350191000
H	7.581205000	-2.259294000	-2.228310000

Entry 6b // Ar*H₂PbPbAr*

Pb	-0.142386000	1.254615000	0.660754000
C	0.048702000	2.939026000	-0.884824000
C	-1.091112000	3.487497000	-1.500346000
C	-0.967691000	4.407556000	-2.546859000
C	0.288581000	4.810499000	-2.984448000
C	1.421603000	4.304430000	-2.357505000
C	1.313556000	3.372422000	-1.315238000
C	2.604470000	2.948514000	-0.676375000
C	3.398765000	1.952978000	-1.266578000
C	4.711339000	1.764344000	-0.811619000
C	5.246056000	2.534196000	0.218094000
C	4.403386000	3.453121000	0.850360000
C	3.092521000	3.670309000	0.434489000
C	-2.451008000	3.164065000	-0.968386000
C	-3.111540000	1.980524000	-1.351328000
C	-4.328140000	1.666624000	-0.752718000
C	-4.909682000	2.488883000	0.215762000
C	-4.240928000	3.652369000	0.577789000
C	-3.016537000	4.006605000	0.001590000
C	-2.296110000	5.249417000	0.506002000
C	-3.202272000	6.485016000	0.512725000
C	-1.706994000	4.996748000	1.900031000
C	-6.244522000	2.084378000	0.813795000
C	-7.383698000	2.427844000	-0.155267000
C	-6.510672000	2.683792000	2.193873000
C	-2.515726000	1.068876000	-2.413118000
C	-2.891373000	-0.400830000	-2.217945000
C	-2.930775000	1.540928000	-3.813021000
C	2.874585000	1.124449000	-2.431193000
C	3.423835000	1.637583000	-3.767895000
C	3.189239000	-0.364928000	-2.267026000
C	6.695579000	2.440321000	0.672048000
C	7.621737000	1.772033000	-0.342828000
C	6.819249000	1.743746000	2.032967000
C	2.237244000	4.720168000	1.127746000
C	2.364550000	4.670056000	2.652670000
C	2.567747000	6.122383000	0.600953000
H	-1.867407000	4.825630000	-2.992709000
H	0.384968000	5.528732000	-3.792999000
H	2.410462000	4.639544000	-2.662322000
H	5.336041000	1.029023000	-1.312815000
H	4.803089000	4.041483000	1.674908000
H	-4.834892000	0.739122000	-1.010015000
H	-4.662274000	4.294465000	1.346481000
H	-1.461428000	5.460307000	-0.168885000
H	-2.626697000	7.373101000	0.793218000
H	-4.020307000	6.383616000	1.233876000
H	-3.642151000	6.657655000	-0.474324000
H	-1.164711000	5.880976000	2.254719000
H	-1.013640000	4.148402000	1.888524000
H	-2.499557000	4.768155000	2.621973000
H	-6.217348000	0.990937000	0.926372000
H	-7.221912000	1.966350000	-1.134747000
H	-7.439635000	3.512407000	-0.300440000

H	-8.347618000	2.082982000	0.235007000
H	-5.676034000	2.497668000	2.877470000
H	-7.416359000	2.247780000	2.626868000
H	-6.666837000	3.766466000	2.132322000
H	-1.421827000	1.153173000	-2.353306000
H	-2.755435000	-0.726054000	-1.174418000
H	-2.296937000	-1.040011000	-2.881422000
H	-3.942760000	-0.591509000	-2.458758000
H	-2.595174000	2.565683000	-3.995415000
H	-4.022248000	1.515264000	-3.909243000
H	-2.500756000	0.894792000	-4.585998000
H	1.782705000	1.237711000	-2.452989000
H	3.131501000	2.676865000	-3.940495000
H	3.047774000	1.032199000	-4.599647000
H	4.518668000	1.585019000	-3.774622000
H	2.914210000	-0.726073000	-1.266725000
H	4.260332000	-0.567763000	-2.384387000
H	2.660097000	-0.958771000	-3.021268000
H	7.041103000	3.474862000	0.804436000
H	7.525325000	2.220144000	-1.336400000
H	7.404879000	0.700830000	-0.427493000
H	8.663389000	1.866933000	-0.021250000
H	6.165108000	2.201922000	2.780846000
H	7.850422000	1.791092000	2.398962000
H	6.542937000	0.686169000	1.946052000
H	1.191026000	4.510159000	0.881004000
H	2.191393000	3.656496000	3.027645000
H	1.625532000	5.336308000	3.109871000
H	3.353699000	4.998804000	2.990112000
H	2.408945000	6.185036000	-0.479773000
H	3.614819000	6.372354000	0.808209000
H	1.934758000	6.873975000	1.085392000
Pb	0.101335000	-1.389536000	-0.813672000
C	-0.105653000	-2.735861000	1.055241000
C	1.078510000	-3.210827000	1.636387000
C	1.031155000	-4.162439000	2.660473000
C	-0.192734000	-4.674159000	3.080027000
C	-1.366274000	-4.256502000	2.458050000
C	-1.334460000	-3.284306000	1.450403000
C	-2.604166000	-2.956813000	0.718599000
C	-3.566219000	-2.085442000	1.277692000
C	-4.791401000	-1.925410000	0.626002000
C	-5.094930000	-2.599332000	-0.558208000
C	-4.111575000	-3.407919000	-1.120731000
C	-2.868006000	-3.599340000	-0.512725000
C	-1.878106000	-4.573266000	-1.143519000
C	-1.862329000	-4.514187000	-2.673842000
H	-1.726644000	-3.488851000	-3.036774000
H	-1.040073000	-5.123472000	-3.061425000
H	-2.787871000	-4.905772000	-3.108056000
C	-2.157203000	-6.003437000	-0.663183000
H	-2.095029000	-6.070052000	0.426845000
H	-3.160398000	-6.319962000	-0.970494000
H	-1.429896000	-6.701652000	-1.092903000
H	-0.872521000	-4.311443000	-0.797959000
H	-4.335239000	-3.923637000	-2.051346000
C	-6.476740000	-2.526669000	-1.183466000
C	-7.492773000	-3.256724000	-0.294849000
H	-7.183292000	-4.289445000	-0.110248000
H	-7.583533000	-2.754373000	0.674689000
H	-8.481855000	-3.268087000	-0.764387000
C	-6.944392000	-1.095657000	-1.460687000
H	-6.263370000	-0.571929000	-2.139367000
H	-7.939236000	-1.100851000	-1.918192000
H	-7.011601000	-0.515294000	-0.533642000
H	-6.426738000	-3.056301000	-2.143559000
H	-5.540332000	-1.273462000	1.070511000
C	-3.311795000	-1.362928000	2.594782000
C	-3.801811000	-2.196867000	3.788238000
H	-3.271796000	-3.146866000	3.875004000
H	-3.656818000	-1.641049000	4.720567000
H	-4.872032000	-2.408639000	3.682035000
C	-3.970931000	0.018918000	2.654026000
H	-3.786152000	0.599724000	1.746306000
H	-5.055050000	-0.065852000	2.800774000
H	-3.572175000	0.583112000	3.503285000
H	-2.227076000	-1.227163000	2.691760000
H	-2.315115000	-4.713352000	2.727446000
H	-0.229871000	-5.429300000	3.859080000
H	1.957864000	-4.537415000	3.088592000
C	2.394935000	-2.859403000	1.006076000
C	3.177636000	-1.764259000	1.442245000
C	4.404019000	-1.533166000	0.822346000
C	4.889415000	-2.347537000	-0.205343000
C	4.099642000	-3.409453000	-0.628452000
C	2.856731000	-3.680168000	-0.044951000
C	2.082194000	-4.903832000	-0.519359000
C	2.806386000	-6.187185000	-0.092915000
H	2.234361000	-7.070142000	-0.396676000
H	3.798426000	-6.248642000	-0.554028000
H	2.936287000	-6.217933000	0.993122000
C	1.840852000	-4.894788000	-2.032516000
H	1.240731000	-5.764675000	-2.322056000
H	1.304282000	-3.992167000	-2.350343000
H	2.780118000	-4.939104000	-2.594199000
H	1.104304000	-4.908031000	-0.028944000
H	4.449050000	-4.054127000	-1.429790000
C	6.240909000	-2.027935000	-0.820137000
C	7.364496000	-2.246859000	0.201954000
H	7.197433000	-1.664740000	1.113426000
H	7.418197000	-3.304188000	0.483396000
H	8.332133000	-1.952986000	-0.218420000

C	6.537123000	-2.794238000	-2.107678000
H	5.745919000	-2.657184000	-2.852095000
H	7.478769000	-2.446336000	-2.542231000
H	6.640450000	-3.867641000	-1.912779000
H	6.222698000	-0.956967000	-1.067791000
H	4.997094000	-0.672678000	1.122301000
C	2.725458000	-0.892705000	2.603970000
C	3.318206000	0.515820000	2.555232000
H	3.199562000	0.979582000	1.570226000
H	2.822285000	1.155524000	3.291551000
H	4.385848000	0.500023000	2.799692000
C	3.087403000	-1.557422000	3.940748000
H	2.600151000	-2.528224000	4.057299000
H	4.171440000	-1.705209000	4.004627000
H	2.779577000	-0.919080000	4.775359000
H	1.631041000	-0.811607000	2.555092000
H	-1.754835000	1.518490000	1.417237000
H	0.942253000	1.810650000	1.977486000

Entry 7b // Ar*HPb-PbHAr*

C	-2.135727000	-2.603198000	-0.225455000
C	-1.315093000	-3.644910000	0.219466000
C	-3.408685000	-2.906297000	-0.729863000
C	-1.762112000	-4.969143000	0.149552000
C	-3.846197000	-4.230159000	-0.823209000
C	-3.017456000	-5.260267000	-0.383381000
H	-1.130098000	-5.772109000	0.522193000
H	-4.840136000	-4.449834000	-1.207649000
H	-3.356184000	-6.290394000	-0.438803000
C	2.199016000	2.549127000	-0.153661000
C	3.416483000	2.699591000	-0.828287000
C	1.443061000	3.680032000	0.170623000
C	3.883140000	3.973837000	-1.159650000
C	1.925775000	4.957403000	-0.137605000
C	3.143352000	5.100238000	-0.798137000
H	4.815874000	4.086917000	-1.706954000
H	1.334660000	5.833818000	0.120219000
H	3.511041000	6.091086000	-1.046988000
C	4.134546000	1.440707000	-1.209281000
C	3.755475000	0.763120000	-2.386811000
C	5.120542000	0.893888000	-0.356777000
C	4.381201000	-0.449869000	-2.694063000
C	5.706287000	-0.324015000	-0.702415000
C	5.351725000	-1.010476000	-1.867746000
H	4.112078000	-0.970434000	-3.611454000
H	6.477115000	-0.740235000	-0.057848000
C	0.095137000	3.457538000	0.784109000
C	-0.020271000	3.016242000	2.119060000
C	-1.061276000	3.577136000	-0.016918000
C	-1.288491000	2.705028000	2.627973000
C	-2.297374000	3.245711000	0.533116000
C	-2.439156000	2.809675000	1.852292000
H	-1.366943000	2.371291000	3.657457000
H	-3.185683000	3.289577000	-0.098055000
C	0.023663000	-3.306633000	0.796576000
C	1.168987000	-3.317425000	-0.026140000
C	0.130730000	-2.901222000	2.139719000
C	2.401973000	-2.985913000	0.534246000
C	1.395897000	-2.612930000	2.669704000
C	2.546071000	-2.671142000	1.889427000
H	3.289562000	-2.962379000	-0.094927000
H	1.473180000	-2.333208000	3.716905000
C	-4.268292000	-1.715170000	-1.042094000
C	-5.115441000	-1.209712000	-0.034529000
C	-4.065272000	-0.974707000	-2.229292000
C	-5.710518000	0.039214000	-0.216143000
C	-4.674820000	0.279715000	-2.358949000
C	-5.487564000	0.810626000	-1.356300000
H	-6.346391000	0.444854000	0.571152000
H	-4.495773000	0.857043000	-3.260141000
C	5.605513000	1.674533000	0.856354000
H	4.787309000	2.330402000	1.175312000
C	2.786622000	1.393463000	-3.380235000
H	2.255450000	2.202134000	-2.868204000
C	-0.995089000	3.990186000	-1.480773000
H	0.017550000	4.341927000	-1.693612000

C	1.187407000	2.996993000	3.050436000
H	2.089327000	2.859633000	2.445305000
C	-3.248033000	-1.568296000	-3.369548000
H	-2.407641000	-2.113511000	-2.925069000
C	-5.352851000	-1.960788000	1.267084000
H	-4.824335000	-2.915862000	1.211580000
C	-1.087685000	-2.807744000	3.047447000
H	-1.983420000	-2.896689000	2.424040000
C	1.074171000	-3.694859000	-1.495494000
H	0.050798000	-3.483175000	-1.825511000
C	-1.953663000	5.144322000	-1.792407000
H	-1.845121000	5.455321000	-2.836454000
H	-2.999695000	4.858199000	-1.639832000
H	-1.747986000	6.008255000	-1.152707000
C	-1.253327000	2.783164000	-2.391055000
H	-2.234786000	2.331959000	-2.187403000
H	-1.228773000	3.078514000	-3.446299000
H	-0.495000000	2.006405000	-2.236240000
C	3.587425000	2.021536000	-4.529729000
H	4.143483000	1.251995000	-5.077376000
H	2.918874000	2.526613000	-5.234631000
H	4.307946000	2.753650000	-4.151668000
C	1.728560000	0.428264000	-3.919910000
H	1.096078000	0.030049000	-3.118955000
H	1.075272000	0.954337000	-4.624778000
H	2.175526000	-0.417420000	-4.454510000
C	2.021862000	-2.878455000	-2.375423000
H	3.070748000	-3.161766000	-2.223714000
H	1.788392000	-3.039859000	-3.433354000
H	1.932071000	-1.808075000	-2.166546000
C	1.338281000	-5.195174000	-1.680180000
H	2.345587000	-5.447018000	-1.327650000
H	0.620276000	-5.798858000	-1.118568000
H	1.266425000	-5.471834000	-2.737413000
C	-1.100401000	-3.971097000	4.046806000
H	-1.098040000	-4.931921000	3.523097000
H	-0.217597000	-3.936735000	4.695325000
H	-1.991483000	-3.926176000	4.681901000
C	-1.167896000	-1.461062000	3.776854000
H	-2.092328000	-1.404072000	4.362765000
H	-0.329780000	-1.321195000	4.468732000
H	-1.162704000	-0.620080000	3.069931000
C	-2.669653000	-0.529604000	-4.331161000
H	-1.986635000	-1.020255000	-5.031475000
H	-3.453944000	-0.046324000	-4.925138000
H	-2.105451000	0.242477000	-3.797373000
C	-4.112588000	-2.580042000	-4.136627000
H	-4.989614000	-2.083064000	-4.566606000
H	-3.539927000	-3.031957000	-4.953261000
H	-4.461305000	-3.381150000	-3.478622000
C	-6.841420000	-2.262948000	1.472090000
H	-7.244280000	-2.839334000	0.633800000
H	-6.990239000	-2.840341000	2.390321000
H	-7.426977000	-1.340978000	1.559007000
C	-4.781839000	-1.184131000	2.457615000
H	-5.315441000	-0.237278000	2.598935000
H	-4.875167000	-1.764836000	3.382323000
H	-3.720755000	-0.950581000	2.303900000
C	1.309653000	4.362207000	3.742120000
H	1.420472000	5.162050000	3.003408000
H	0.414057000	4.569531000	4.338705000
H	2.179527000	4.383045000	4.406990000
C	1.152259000	1.869273000	4.086506000
H	2.115262000	1.813210000	4.603775000
H	0.379573000	2.034475000	4.845398000
H	0.965535000	0.891134000	3.625111000
C	6.795339000	2.557388000	0.452107000
H	7.137505000	3.156431000	1.302529000
H	7.631012000	1.934175000	0.113443000
H	6.530423000	3.237399000	-0.362004000
C	5.982793000	0.801435000	2.053212000
H	6.845290000	0.159590000	1.840923000
H	6.254659000	1.437713000	2.901773000
H	5.142285000	0.172504000	2.356063000
H	2.870643000	0.440448000	1.824857000
H	-0.801360000	-0.467451000	-1.865260000
Pb	-1.649936000	-0.311141000	-0.195101000
Pb	1.538375000	0.434827000	0.528832000
C	-6.161971000	2.167207000	-1.470533000
H	-6.066647000	2.652164000	-0.487881000
C	-7.658863000	1.989269000	-1.761793000
H	-8.165730000	2.959073000	-1.799712000
H	-7.795756000	1.491970000	-2.728277000
H	-8.144291000	1.375821000	-0.997169000
C	-5.527912000	3.087015000	-2.512842000
H	-5.710099000	2.718792000	-3.528631000
H	-5.960952000	4.089653000	-2.445153000
H	-4.444736000	3.171062000	-2.375909000
C	-3.824783000	2.454242000	2.366328000
H	-4.230977000	1.700361000	1.672463000
C	-3.821065000	1.854163000	3.770534000
H	-4.837894000	1.580447000	4.068220000
H	-3.198399000	0.955140000	3.827352000
H	-3.447220000	2.578751000	4.503214000
C	-4.750187000	3.678771000	2.325323000
H	-4.790364000	4.126079000	1.327673000
H	-5.769093000	3.400863000	2.615931000
H	-4.393643000	4.446453000	3.021007000
C	3.941404000	-2.425515000	2.434030000
H	4.448073000	-1.764786000	1.714147000
C	4.721831000	-3.747473000	2.484226000
H	5.752732000	-3.574933000	2.811991000

H	4.248953000	-4.439724000	3.189795000
H	4.749355000	-4.233694000	1.504426000
C	3.961958000	-1.752093000	3.804287000
H	4.992247000	-1.526269000	4.097226000
H	3.393351000	-0.815836000	3.800290000
H	3.539904000	-2.411998000	4.571060000
C	6.073225000	-2.283109000	-2.274803000
H	5.552947000	-2.686888000	-3.153464000
C	6.058423000	-3.358728000	-1.184259000
H	6.629539000	-4.235877000	-1.505567000
H	6.507445000	-2.991710000	-0.254452000
H	5.039351000	-3.687283000	-0.958213000
C	7.515681000	-1.959753000	-2.687402000
H	8.027491000	-2.857954000	-3.048091000
H	7.537789000	-1.205046000	-3.478774000
H	8.079809000	-1.568031000	-1.833592000

Entry 8b // Ar*Pb(μ-H)₂PbAr*

Pb	0.055776000	-1.382274000	-0.952779000
C	-0.132953000	-4.467653000	3.164328000
H	-0.177503000	-5.148384000	4.009066000
C	-0.020866000	-2.705381000	0.966938000
C	1.155656000	-3.169933000	1.578118000
C	-1.302936000	-4.055616000	2.535082000
H	-2.266229000	-4.432007000	2.871446000
C	-1.253705000	-3.184139000	1.438816000
C	-2.550156000	-2.883481000	0.744922000
C	-3.444510000	-1.928648000	1.272804000
C	-4.727176000	-1.828627000	0.729785000
H	-5.427114000	-1.114422000	1.161602000
C	-5.147710000	-2.647963000	-0.321275000
C	-6.588732000	-2.656652000	-0.800222000
H	-6.638457000	-3.332248000	-1.663784000
C	-7.503574000	-3.223080000	0.293704000
H	-7.495413000	-2.571924000	1.175059000
H	-7.171609000	-4.216706000	0.607942000
H	-8.536356000	-3.297193000	-0.062671000
C	-7.089661000	-1.283036000	-1.251777000
H	-6.481331000	-0.881834000	-2.068617000
H	-7.065237000	-0.565407000	-0.424463000
H	-8.125760000	-1.348016000	-1.600529000
C	-4.219769000	-3.521999000	-0.880664000
H	-4.530401000	-4.144139000	-1.717257000
C	-2.921647000	-3.649479000	-0.378288000
C	-1.976844000	-4.671074000	-0.999028000
H	-0.955151000	-4.415046000	-0.697637000
C	-2.269034000	-6.074303000	-0.453775000
H	-3.288844000	-6.381220000	-0.712801000
H	-2.170980000	-6.096308000	0.635764000
H	-1.572226000	-6.805942000	-0.877764000
C	-2.014917000	-4.6611352000	-2.530260000
H	-1.855133000	-3.652643000	-2.927796000
H	-2.971576000	-5.026907000	-2.917718000
H	-1.230932000	-5.313520000	-2.928449000
C	-3.043096000	-1.054883000	2.453051000
H	-1.949097000	-1.088918000	2.528533000
C	-3.624322000	-1.603438000	3.762706000
H	-3.274210000	-2.619799000	3.961711000
H	-4.719201000	-1.623977000	3.713134000
H	-3.333641000	-0.969773000	4.607333000
C	-3.451838000	0.408815000	2.267165000
H	-4.539928000	0.535308000	2.325738000
H	-3.131299000	0.794329000	1.294000000
H	-3.011301000	1.028495000	3.057260000
C	2.496543000	-2.861755000	0.983548000
C	3.272336000	1.776497000	1.446773000
C	4.529149000	-1.564527000	0.888662000
H	5.123551000	-0.717228000	1.222724000
C	5.046669000	-2.388187000	-0.117116000
C	6.429620000	-2.090826000	-0.671172000
H	6.450236000	-1.015664000	-0.904316000
C	6.759624000	-2.844329000	-1.958223000
H	6.001001000	-2.676719000	-2.729761000
H	6.829335000	-3.922664000	-1.776521000

H	7.726010000	-2.513597000	-2.350195000
C	7.501611000	-2.357373000	0.394120000
H	7.520213000	-3.422626000	0.649230000
H	7.301690000	-1.796191000	1.312106000
H	8.493965000	-2.073789000	0.027430000
C	4.260436000	-3.439534000	-0.570792000
H	4.632105000	-4.089269000	-1.358466000
C	2.989888000	-3.692794000	-0.037428000
C	2.209485000	-4.896965000	-0.548736000
H	1.243262000	-4.924278000	-0.036028000
C	2.941244000	-6.200495000	-0.206308000
H	3.107470000	-6.280247000	0.872268000
H	2.354845000	-7.066871000	-0.529935000
H	3.916856000	-6.248036000	-0.702586000
C	1.932693000	-4.808161000	-2.053405000
H	1.367336000	-3.902641000	-2.305871000
H	1.348622000	-5.673913000	-2.384874000
H	2.862102000	-4.789344000	-2.633158000
C	2.762071000	-0.878532000	2.562073000
H	1.665147000	-0.907629000	2.528672000
C	3.204112000	0.578202000	2.407813000
H	3.047948000	0.944587000	1.387298000
H	4.267600000	0.705900000	2.640068000
H	2.648375000	1.215807000	3.105485000
C	3.201659000	-1.417688000	3.930398000
H	4.295707000	-1.451570000	3.987550000
H	2.819074000	-2.426561000	4.105301000
H	2.836766000	-0.769078000	4.734041000
H	1.228798000	0.016662000	0.032749000
C	1.095720000	-4.036539000	2.675600000
H	2.019739000	-4.401314000	3.117982000
Pb	-0.055776000	1.382274000	0.952779000
C	0.132954000	4.467649000	-3.164331000
H	0.177504000	5.148378000	-4.009071000
C	0.020867000	2.705380000	-0.966939000
C	-1.155656000	3.169931000	-1.578121000
C	1.302937000	4.055613000	-2.535084000
H	2.266230000	4.432004000	-2.871449000
C	1.253706000	3.184138000	-1.438817000
C	2.550156000	2.883481000	-0.744921000
C	3.444511000	1.928649000	-1.272804000
C	4.727177000	1.828628000	-0.729783000
H	5.427116000	1.114425000	-1.161600000
C	5.147708000	2.647964000	0.321278000
C	6.588730000	2.656653000	0.800227000
H	6.638453000	3.332248000	1.663791000
C	7.503573000	3.223085000	-0.293696000
H	7.495414000	2.571931000	-1.175053000
H	7.171607000	4.216712000	-0.607932000
H	8.536354000	3.297199000	0.062680000
C	7.089660000	1.283037000	1.251780000
H	6.481329000	0.881832000	2.068618000
H	7.065238000	0.565410000	0.424464000
H	8.125758000	1.348017000	1.600533000
C	4.219767000	3.521999000	0.880667000
H	4.530396000	4.144138000	1.717261000
C	2.921645000	3.649478000	0.378289000
C	1.976840000	4.671072000	0.999029000
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C	2.269022000	6.074300000	0.453771000
H	3.288832000	6.381222000	0.712793000
H	2.170966000	6.096302000	-0.635767000
H	1.572213000	6.805937000	0.877760000
C	2.014917000	4.661355000	2.530260000
H	1.855140000	3.652645000	2.927800000
H	2.971574000	5.026917000	2.917716000
H	1.230929000	5.313519000	2.928449000
C	3.043099000	1.054884000	-2.453051000
H	1.949101000	1.088920000	-2.528536000
C	3.624329000	1.603438000	-3.762705000
H	3.274217000	2.619800000	-3.961711000
H	4.719207000	1.623978000	-3.713131000
H	3.333650000	0.969774000	-4.607333000
C	3.451841000	-0.408814000	-2.267165000
H	4.539930000	-0.535308000	-2.325735000
H	3.131299000	-0.794328000	-1.294000000
H	3.011305000	-1.028493000	-3.057261000
C	-2.496543000	2.861754000	-0.983549000
C	-3.272336000	1.776496000	-1.446774000
C	-4.529149000	1.564527000	-0.888661000
H	-5.123551000	0.717227000	-1.222722000
C	-5.046668000	2.388188000	0.117116000
C	-6.429618000	2.090827000	0.671174000
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C	-6.759621000	2.844331000	1.958224000
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H	-6.829333000	3.922666000	1.776522000
H	-7.726007000	2.513599000	2.350197000
C	-7.501611000	2.357375000	-0.394118000
H	-7.520212000	3.422628000	-0.649228000
H	-7.301691000	1.796192000	-1.312104000
H	-8.493965000	2.073791000	-0.027427000
C	-4.260434000	3.439535000	0.570791000
H	-4.632103000	4.089270000	1.358465000
C	-2.989886000	3.692794000	0.037426000
C	-2.209483000	4.896966000	0.548733000
H	-1.243260000	4.924277000	0.036025000
C	-2.941242000	6.200495000	0.206302000
H	-3.107468000	6.280246000	-0.872274000
H	-2.354842000	7.066871000	0.529929000
H	-3.916853000	6.248038000	0.702580000
C	-1.932691000	4.808163000	2.053402000

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H   -1.367335000   3.902644000   2.305869000
H   -1.348619000   5.673915000   2.384869000
H   -2.862100000   4.789349000   2.633155000
C   -2.762072000   0.878530000   -2.562073000
H   -1.665149000   0.907627000   -2.528674000
C   -3.204113000   -0.578203000   -2.407812000
H   -3.047949000   -0.944588000   -1.387297000
H   -4.267602000   -0.705901000   -2.640066000
H   -2.648377000   -1.215809000   -3.105485000
C   -3.201661000   1.417686000   -3.930398000
H   -4.295710000   1.451568000   -3.987549000
H   -2.819077000   2.426559000   -4.105303000
H   -2.836770000   0.769075000   -4.734041000
H   -1.228798000   -0.016662000   -0.032749000
C   -1.095720000   4.036535000   -2.675603000
H   -2.019738000   4.401310000   -3.117986000

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