Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information for

Palladium-Catalysed Magnesiation of Benzene

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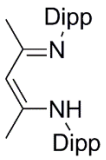
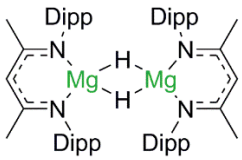
Contents

1. General experimental

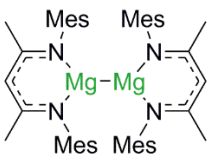
Unless otherwise specified, all manipulations were carried out using standard Schlenk and glovebox techniques, under inert atmosphere (nitrogen or argon). A MBRAUN Labmaster glovebox was employed operating with concentrations of H_2O and O_2 below 0.1 ppm. Anhydrous solvents were obtained from a Grubbs 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] ^{Dipp}BDIMgH,[2] ^{Mes}BDIMg-MgBDI^{Mes} **1a**,[3] and [$PdMe_2$(TMEDA)][4] were prepared by literature procedures (BDI = β-diketiminate, see below for structures of these starting materials). [$Pd(PCy_3)_2$] was synthesised by modified literature procedures due to the insufficient purity of commercial samples.



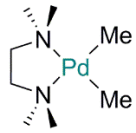
^{Dipp}BDIH



^{Dipp}BDIMgH



^{Mes}BDIMgMgBDI^{Mes}



$PdMe_2$(TMEDA)

(Dipp = 2,6-diisopropylphenyl)
(Mes = 2,4,6-trimethylphenyl)

^{1}H-, ^{13}C-, and ^{31}P-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).

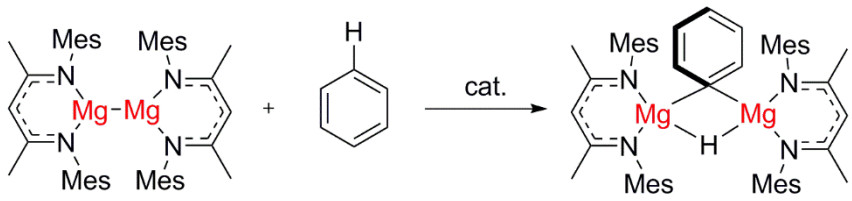
Single crystal X-Ray data was obtained on Agilent Diffraction Xcalibur PX Ultra A and Xcalibur 3 E diffractometers, and the structures were refined using the SHELXTL and SHELX-2013 program systems.[5]

2. Experimental procedures

2.1. Synthesis of $[Pd(PCy_3)_2]$.[6]

A NaCp (357 mg, 4.05 mmol, 1.05 equiv.) solution in dry THF (20 mL) was added *via* cannula to a suspension of $[PdCl(\pi\text{-cinnamyl})]_2$ (1000 mg, 1.93 mmol, 0.5 equiv.) in dry THF (20 mL) at 0°C. The reaction mixture was stirred at 25°C for 1h. Volatiles were then removed *in vacuo*. Hexane (5 mL) was added and subsequently evaporated to remove THF traces. Hexane (30 mL) was added and the mixture was filtered *via* cannula to remove NaCl and insoluble impurities. The solvent was then removed *in vacuo* and recrystallised from hexane to afford [PdCp(π-cinnamyl)] as a dark red crystalline solid (702 mg, 63%). The product was used in the next step without further purification. A PCy_3 (1069 mg, 3.81 mmol, 2.2 equiv.) solution in dry toluene (15 mL) was added to [PdCp(π-cinnamyl)] (500 mg, 1.73 mmol, 1 equiv.). The reaction mixture was stirred at 80°C for 3h. The volatiles were then evaporated and the brown solid was washed with dry MeOH (2x8mL). The solid was then dried *in vacuo*, dissolved in hot toluene (5 mL) and layered with MeOH (10 mL). The product was left in the freezer overnight. The crystals were then isolated by filtration, washed twice with MeOH and dried *in vacuo* to afford $[Pd(PCy_3)_2]$ as pale white-orange crystals (1070 mg, 93%). ^{1}H-NMR (400 MHz, C_6D_6) δ (ppm): 1.17–1.35 (m, 9H), 1.59–1.75 (m, 9H), 1.76–1.90 (m, 9H), 2.15–2.26 (m, 6H). ^{31}P-{^{1}H}-NMR (162 MHz, C_6D_6) δ (ppm): 39.06 (s). Data are consistent with those previously reported.[7]

Table S1. Comparison of catalysts for formation of **2** from **1a**



Catalyst	Conditions	Conversion to 2	Comments
10 mol% $PdMe_2(TMEDA)$	1 day 25°C, 1 day 50°C	57%	Low purity, several by-products generated
5% $Ni(COD)_2$ / 10% PCy_3	4 days, 80°C	62%	Prolonged heating required to generate the product. Low purity
5 mol% $Pt(PCy_3)_2$	3 days, 50°C	35%	Good purity, but low activity
5 mol% $Pd(PCy_3)_2$	2 days, 25°C	Full conversion	Good purity

3. Kinetics

Both reactions showed a first-order type behaviour and plateaued at 71-72% yield of product. Kinetic profiles are very similar, without major isotope effects.

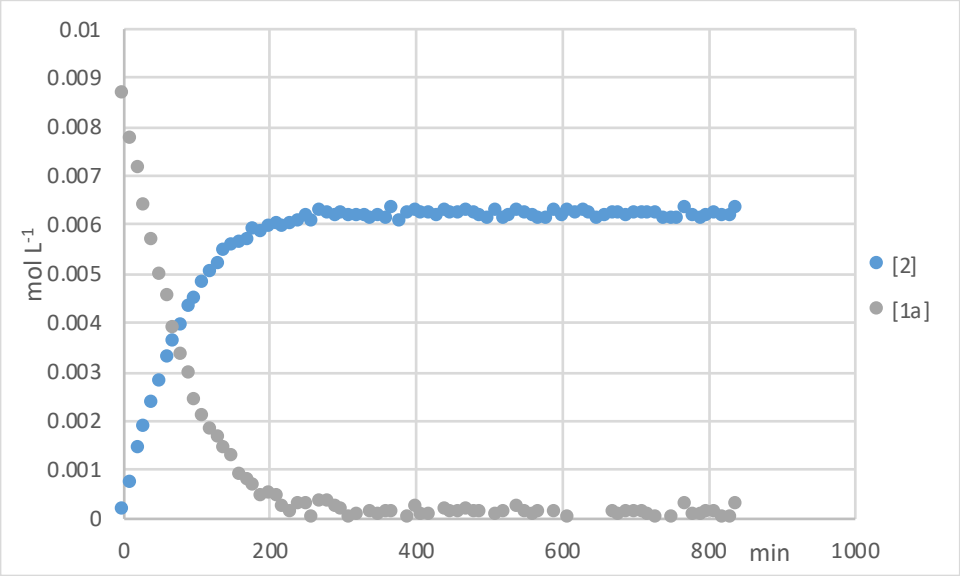


Fig. S1. Plot of the concentration vs time for the reaction between the Mg(I) dimer **1a** and C_6H_6.

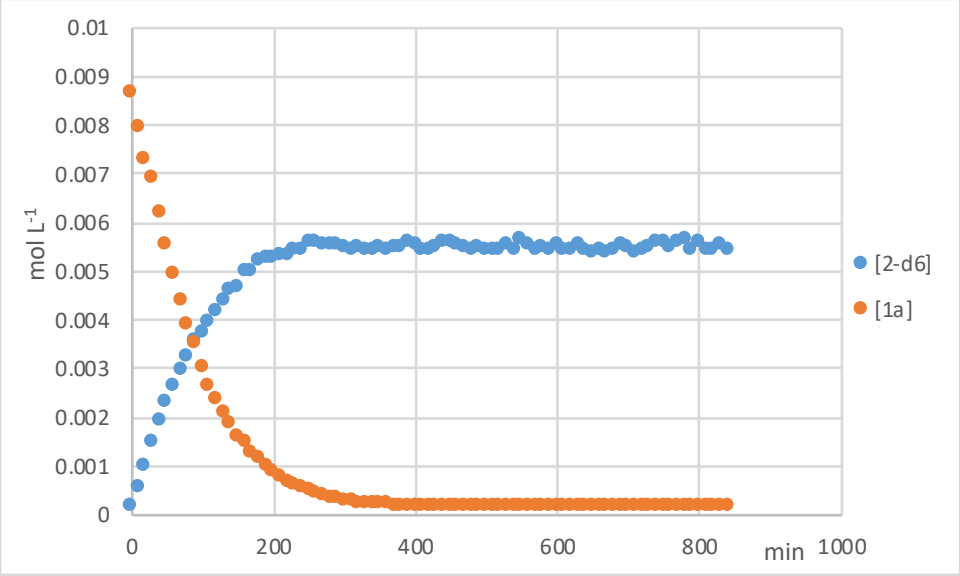


Fig. S2. Plot of the concentration vs time for the reaction between the Mg(I) dimer **1a** and C_6D_6.

The kinetic data was calculated by monitoring the consumption of the starting material **1**. The data was fitted to the highest conversion possible before exiting the linear regime. For C6D6, linearity was maintained until 4.5 lifetimes (96% conversion). For C6H6, probably due to the difficulty to integrate accurately small signals in non-deuterated solvents, linearity was maintained until practically 3 lifetimes (86% conversion).

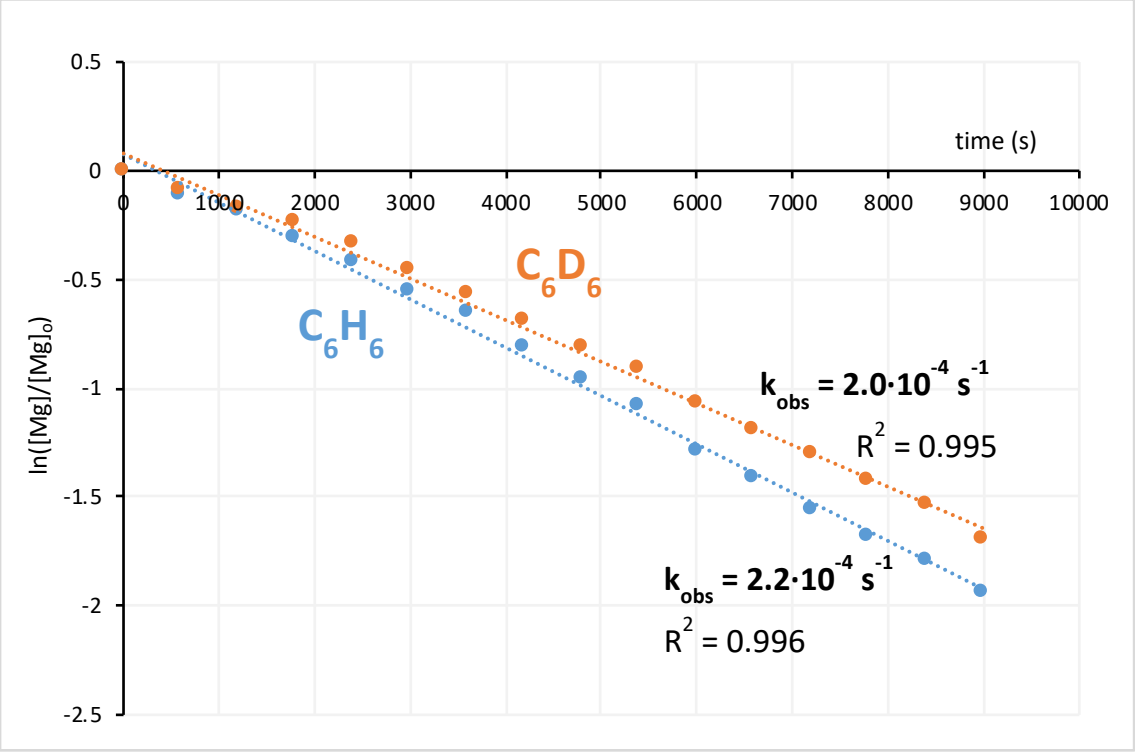


Fig. S3. Linear plots for the kinetics of the reactions between **1** and C_6H_6 and C_6D_6, respectively.

From this data, a k_H/k_D = 1.1 can be derived.

4. Selected multinuclear NMR data

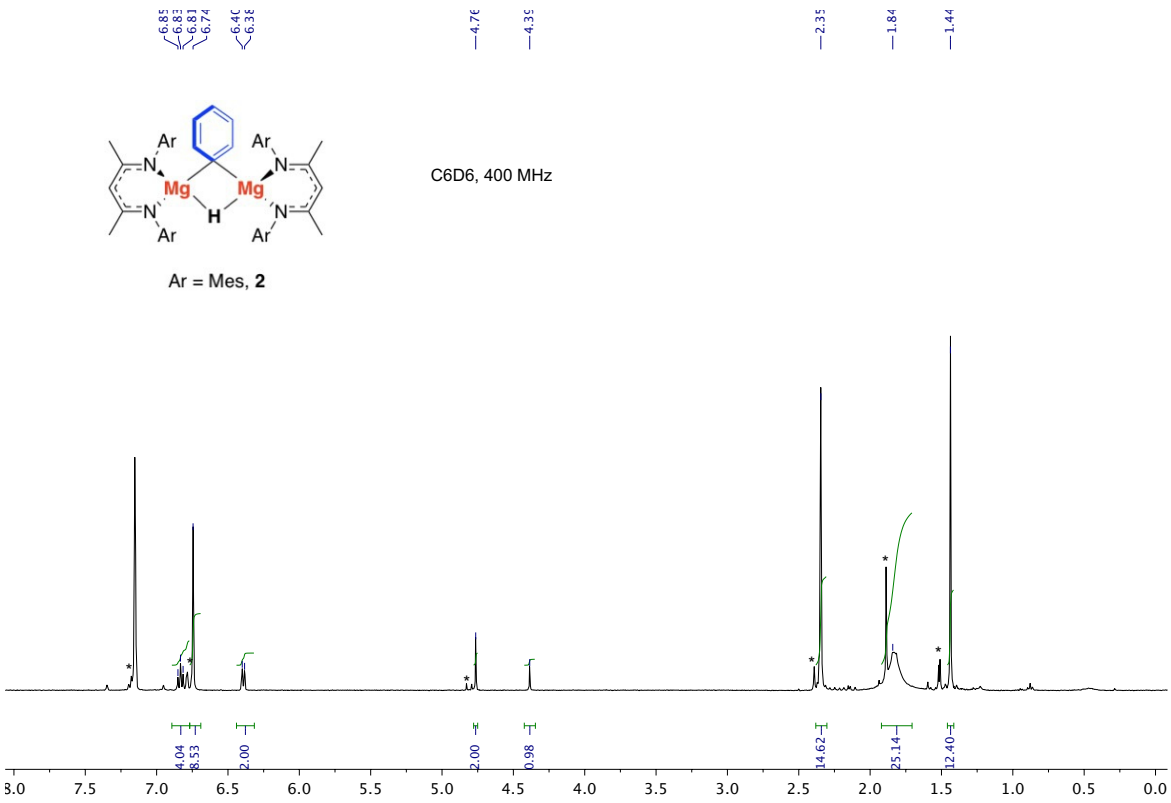


Fig. S4. ^{1}H NMR data for **2**. Peaks marked with a * are an impurity, *i.e.* the corresponding dimeric magnesium hydroxide [^{Mes}BDIMgOH]$_2$.

5. X-ray crystallographic data

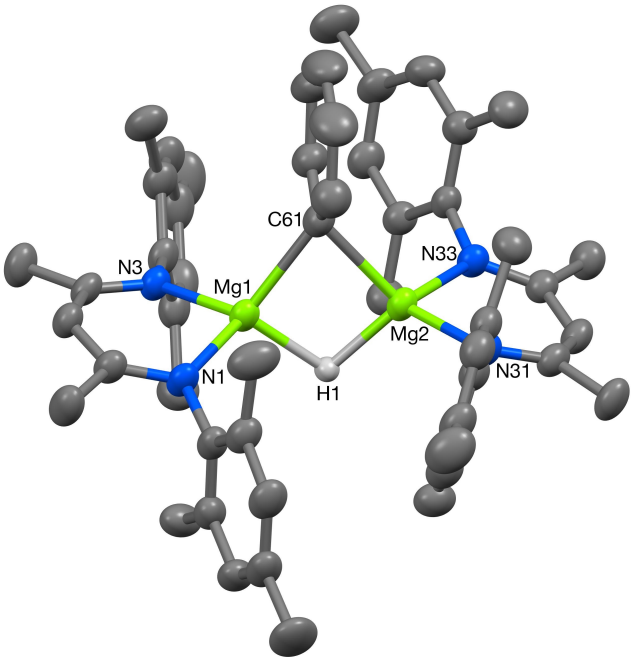


Fig. S5. The crystal structure of **2** (50% probability ellipsoids).

The X-ray crystal structure of 2

Crystal data for **2**: $C_{52}H_{64}Mg_2N_4$, M = 793.69, triclinic, P-1 (no. 2), a = 10.5161(7), b = 13.6510(7), c = 17.9616(18) Å, α = 78.981(6), β = 77.249(7), γ = 69.307(6)°, V = 2334.5(3) Å^3, Z = 2, D_c = 1.129 g cm^{-3}, μ(Cu-Kα) = 0.739 mm^{-1}, T = 173 K, colourless thin plates, Agilent Xcalibur PX Ultra A diffractometer; 8874 independent measured reflections (R_{int} = 0.0402), F^2 refinement,[X1,X2] R_1(obs) = 0.0604, wR_2(all) = 0.1843, 6189 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$], completeness to θ_{full}(67.7°) = 98.0%], 542 parameters. CCDC 1858121.

The Mg–H–Mg bridging hydride atom in the structure of **2** was located from a ΔF map and refined freely with a fixed isotropic thermal parameter of 0.05. When allowed to refine, the thermal parameter of this hydrogen atom went negative, suggesting the presence of more electron density at this site than just a hydrogen atom. The most likely explanation is the co-crystallisation of a small amount (less than *ca*. 10%) of the bridging hydroxy species. However, attempts to model this provided no significant benefits so the simpler model was retained with the thermal parameter of the bridging hydride fixed at 0.05. As a result of this likely co-crystallisation, bond lengths and angles involving this hydrogen atom should be treated with more caution than normal.

6. DFT calculations

6.1. Methods

The geometries of products were optimised with the ωB97x hybrid exchange-correlation DFT functional using the Gaussian09 program package.[8] 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.[9] QTAIM analysis was conducted with the AIMAll package.[10]

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*
****
3 0 *(atom 3 is the hydride)*
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).

6.2. QTAIM analysis

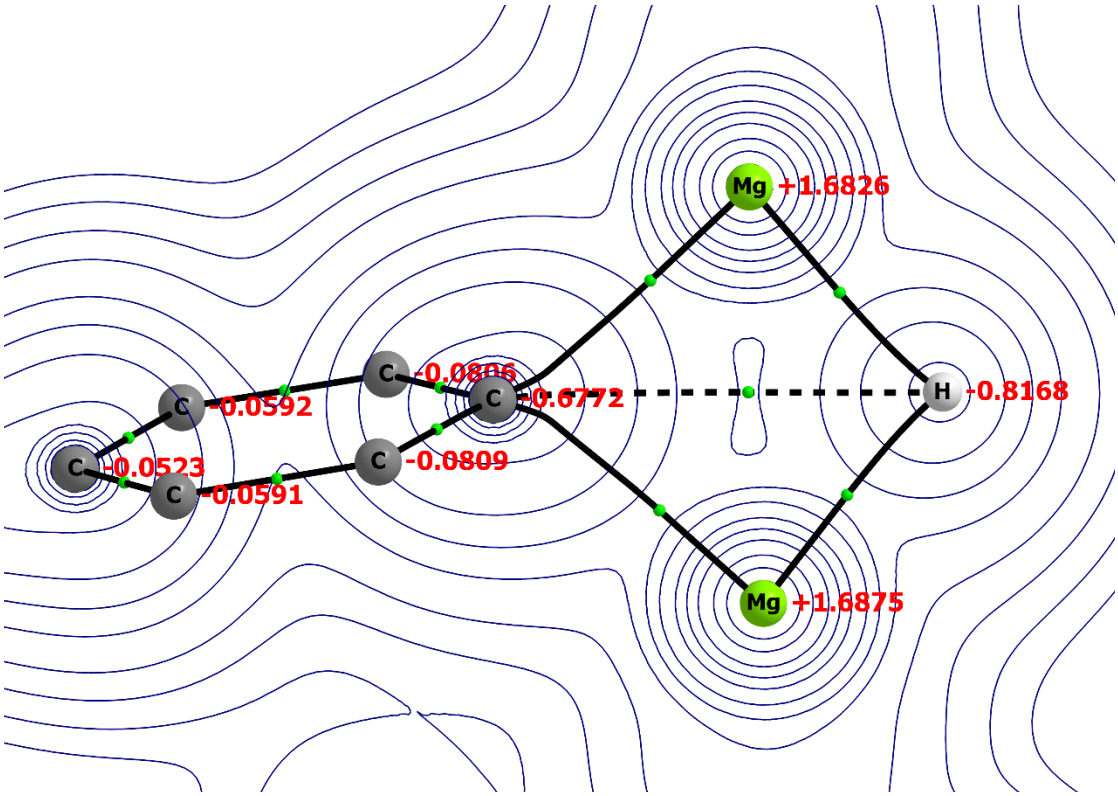


Fig. S6. QTAIM contour plot of ρ for **2**. The ligands on Mg and selected hydrogens have been omitted for clarity. Charges are depicted in red.

Table S2. Values of electron density (ρ), the Laplacian of ρ ($\nabla^2\rho$) and the energy density (H) for selected bond critical points (bcp).

	ρ	$\nabla^2\rho$	H
Mg–H	0.03	0.14-0.15	-0.006
Mg–C_{ipso}	0.03-0.04	0.15-0.17	-0.005
C_{ipso}–H	0.02	0.02	-0.002

6.3. NBO analysis

Table S3. Selected Wiberg Bond Indices (WBI) of **2.**

	2
Mg(1)-H	0.14
Mg(2)-H	0.16
Mg(1)-Mg(2)	0.02
Mg(1)-C_{ipso}	0.11
Mg(2)-C_{ipso}	0.09
C_{ipso}-H	0.02

Table S4. Selected *NPA* charges of **2**.

	Mg(1)	**Mg(2)**	**C_{ipso}**	**H**
2	1.72	1.73	-0.84	-0.80

6.4. Thermochemistry

For the sake of comparison, the thermochemistries of the reactions between benzene and **1a** and **1a-H_2**, respectively, were compared to the analogous reactions previously reported by our group using Al reagents.[11] The same trend was observed. Using low valent complexes, *i.e.* Mg(I) or Al(I), results in a thermodynamically favourable process, whereas using the hydride complexes results in an endergonic process.

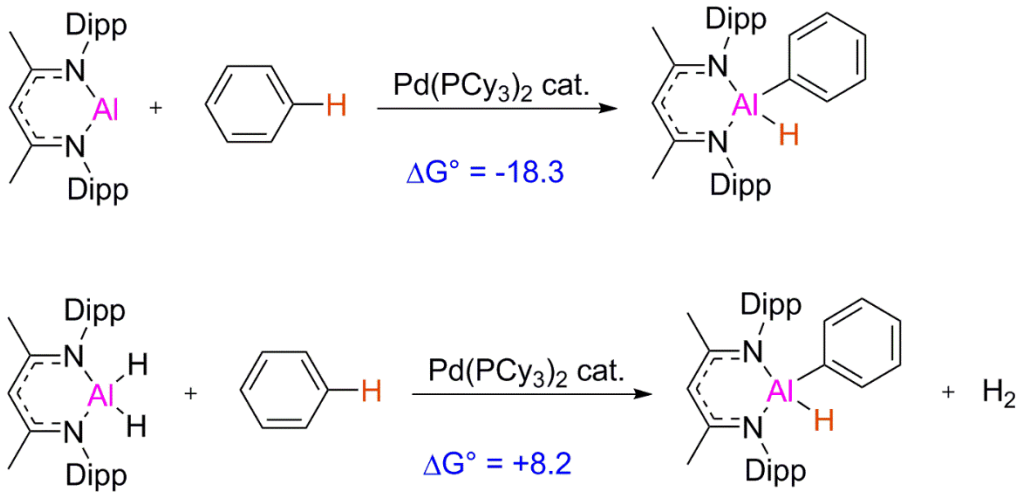


Fig. S7. Calculated energies for the reactions between Al reagents and benzene. Energies (in kcal·mol^{-1}) were calculated at the ωB97x level.

7. XYZ coordinates

benzene.log

SCF (wB97x) = -232.178705763
E(SCF)+ZPE(0 K) = -232.076585
H(298 K)= -232.071306
G(298 K)= -232.103365
Lowest Frequency = 418.3995 cm^{-1}

C	0.307056	0.455804	-3.547102
C	-0.846101	0.102005	-2.852079
C	1.460214	0.809602	-2.852079
H	-1.745864	-0.174047	-3.396300
H	2.359977	1.085654	-3.396300
C	-0.846146	0.101991	-1.459583
C	1.460258	0.809616	-1.459583
H	-1.746444	-0.174224	-0.916212
H	2.360557	1.085831	-0.916212
C	0.307056	0.455804	-0.763390
H	0.307056	0.455804	0.323896
H	0.307056	0.455804	-4.633909

CH4.log

SCF (wB97x) = -40.5008151207
E(SCF)+ZPE(0 K) = -40.455272
H(298 K)= -40.451463
G(298 K)= -40.474939
Lowest Frequency = 1366.9420 cm^{-1}

C	0.064472	1.246805	-0.000001
H	0.427643	0.216726	0.000002
H	0.427663	1.761833	0.892071
H	0.427663	1.761836	-0.892071
H	-1.027747	1.246815	0.000000

H2.log

SCF (wB97x) = -1.17163545979
E(SCF)+ZPE(0 K)= -1.161514
H(298 K)= -1.158209
G(298 K)= -1.173005
Lowest Frequency = 4442.7596 cm^{-1}

H	0.000000	0.000000	0.127869
H	0.000000	0.000000	0.872131

MgHMeMg.log

SCF (wB97x) = -2048.77260214
E(SCF)+ZPE(0 K)= -2047.782165
H(298 K)= -2047.720904
G(298 K)= -2047.877417
Lowest Frequency = 14.2329 cm^{-1}

Mg	-0.000039	-1.424309	0.131425
Mg	0.000031	1.333506	-0.270036
H	0.000021	-0.232393	-1.333113
N	1.504991	-2.814605	0.230224
C	1.273751	-4.098874	0.479786
C	-0.000073	-4.673379	0.650809
H	-0.000085	-5.735101	0.868051
C	-1.273883	-4.098853	0.479751
N	-1.505095	-2.814577	0.230196
C	2.443256	-5.062225	0.563268
H	2.977251	-5.099965	-0.392792
H	2.104740	-6.069606	0.812362
H	3.170057	-4.738487	1.315239
C	-2.443404	-5.062187	0.563188
H	-3.170214	-4.738459	1.315154
H	-2.104909	-6.069581	0.812261
H	-2.977382	-5.099893	-0.392883
C	2.860968	-2.432959	-0.022194
C	3.344709	-2.449088	-1.339865
C	4.686283	-2.144876	-1.568478
H	5.064463	-2.172104	-2.590536
C	5.554195	-1.822398	-0.527071
C	5.035562	-1.763711	0.764675
H	5.690359	-1.486004	1.590474
C	3.699129	-2.052065	1.036985
C	2.431992	-2.809987	-2.485159
H	2.018980	-3.820138	-2.374026
H	2.968124	-2.765159	-3.438282
H	1.577481	-2.123597	-2.543129
C	7.015340	-1.554615	-0.791857
H	7.164783	-1.079417	-1.768031
H	7.593928	-2.486640	-0.791793
H	7.446844	-0.900385	-0.026514
C	3.171128	-1.974669	2.447515
H	2.373797	-1.226529	2.529789
H	3.967028	-1.694509	3.144270
H	2.746920	-2.929645	2.780331
C	-2.861063	-2.432902	-0.022232
C	-3.699235	-2.052034	1.036949
C	-5.035658	-1.763646	0.764628
H	-5.690463	-1.485960	1.590427
C	-5.554270	-1.822271	-0.527130
C	-4.686348	-2.144727	-1.568534
H	-5.064511	-2.171908	-2.590599
C	-3.344783	-2.448975	-1.339910
C	-3.171256	-1.974698	2.447490
H	-2.747068	-2.929693	2.780279
H	-3.967163	-1.694550	3.144243
H	-2.373914	-1.226574	2.529804
C	-7.015405	-1.554443	-0.791928
H	-7.164829	-1.079280	-1.768121
H	-7.446885	-0.900164	-0.026613
H	-7.594029	-2.486446	-0.791823
C	-2.432056	-2.809852	-2.485203
H	-1.577536	-2.123470	-2.543144
H	-2.968176	-2.764992	-3.438331
H	-2.019056	-3.820011	-2.374092
N	1.483021	2.722274	-0.526790
C	1.268435	3.878952	-1.141754
C	0.000064	4.366251	-1.511426

H	0.000074	5.312920	-2.039607
C	-1.268317	3.878987	-1.141737
N	-1.482924	2.722314	-0.526777
C	2.444730	4.785793	-1.448143
H	2.900731	5.147626	-0.519600
H	2.131564	5.649065	-2.038627
H	3.226619	4.247402	-1.993304
C	-2.444590	4.785865	-1.448101
H	-3.226505	4.247500	-1.993251
H	-2.131409	5.649131	-2.038585
H	-2.900564	5.147705	-0.519547
C	2.801863	2.449876	-0.049537
C	3.170978	2.891487	1.231572
C	4.461061	2.627042	1.688609
H	4.750334	2.976457	2.679565
C	5.390532	1.943974	0.906798
C	4.993860	1.507903	-0.355578
H	5.705412	0.973556	-0.982999
C	3.707292	1.731168	-0.843956
C	2.196732	3.664143	2.086225
H	1.898716	4.608039	1.613076
H	2.635900	3.898335	3.060917
H	1.273292	3.097185	2.256151
C	6.778053	1.659137	1.425665
H	6.812824	0.695646	1.951250
H	7.107249	2.428030	2.132578
H	7.507767	1.614569	0.609783
C	3.304989	1.234819	-2.210538
H	2.437885	0.564837	-2.152572
H	4.124588	0.679316	-2.676563
H	3.023535	2.059409	-2.877314
C	-2.801766	2.449941	-0.049509
C	-3.707221	1.731262	-0.843925
C	-4.993785	1.508012	-0.355529
H	-5.705356	0.973686	-0.982946
C	-5.390427	1.944069	0.906861
C	-4.460932	2.627111	1.688666
H	-4.750183	2.976515	2.679633
C	-3.170852	2.891541	1.231612
C	-3.304947	1.234927	-2.210521
H	-3.023490	2.059523	-2.877289
H	-4.124562	0.679445	-2.676541
H	-2.437853	0.564931	-2.152577
C	-6.777945	1.659246	1.425745
H	-7.507683	1.614771	0.609880
H	-7.107091	2.428096	2.132728
H	-6.812739	0.695715	1.951254
C	-2.196577	3.664161	2.086263
H	-1.273163	3.097163	2.256199
H	-2.635739	3.898379	3.060951
H	-1.898517	4.608041	1.613108
C	-0.000071	0.226094	1.703619
H	-0.882796	0.785932	2.059961
H	0.882570	0.786009	2.060048
H	-0.000056	-0.662410	2.359523

2.log

SCF (wB97x) = -2240.46393212
E(SCF)+ZPE(0 K)= -2239.416969

H(298 K)= -2239.353260
G(298 K)= -2239.513909
Lowest Frequency = 17.8789 cm^{-1}

Mg	0.000029	1.519020	-0.240281
Mg	-0.000020	-1.333486	-0.663060
H	0.000023	0.263279	-1.690919
N	-1.510273	2.931712	-0.230561
C	-1.274093	4.238339	-0.292073
C	0.000063	4.832841	-0.322422
H	0.000075	5.915104	-0.374513
C	1.274207	4.238311	-0.292086
N	1.510361	2.931679	-0.230574
C	-2.442893	5.206630	-0.343471
H	-3.076530	5.006812	-1.214159
H	-2.092801	6.238998	-0.397399
H	-3.081513	5.100465	0.539474
C	2.443027	5.206578	-0.343501
H	3.081662	5.100398	0.539430
H	2.092955	6.238954	-0.397420
H	3.076641	5.006749	-1.214203
C	-2.884538	2.532034	-0.210042
C	-3.552097	2.285324	-1.422548
C	-4.913573	1.993685	-1.392143
H	-5.437935	1.834622	-2.335111
C	-5.626219	1.920213	-0.194211
C	-4.929987	2.117981	0.994398
H	-5.464917	2.059569	1.942242
C	-3.567909	2.429100	1.010301
C	-2.818248	2.400279	-2.735451
H	-2.491164	3.430657	-2.924720
H	-3.458861	2.091683	-3.567727
H	-1.915816	1.777532	-2.748724
C	-7.110400	1.648526	-0.199951
H	-7.340117	0.660459	-0.617778
H	-7.644017	2.388823	-0.807139
H	-7.525834	1.683304	0.812473
C	-2.868951	2.727329	2.313376
H	-1.922232	2.184719	2.400651
H	-3.500398	2.452188	3.164108
H	-2.631554	3.795300	2.404146
C	2.884618	2.531974	-0.210067
C	3.568001	2.429038	1.010270
C	4.930074	2.117897	0.994354
H	5.465015	2.059488	1.942192
C	5.626289	1.920104	-0.194261
C	4.913631	1.993576	-1.392186
H	5.437979	1.834494	-2.335159
C	3.552160	2.285241	-1.422578
C	2.869064	2.727288	2.313350
H	2.631676	3.795262	2.404113
H	3.500521	2.452151	3.164077
H	1.922341	2.184688	2.400644
C	7.110464	1.648385	-0.200015
H	7.340153	0.660291	-0.617796
H	7.525918	1.683206	0.812400
H	7.644086	2.388639	-0.807250
C	2.818298	2.400196	-2.735474
H	1.915867	1.777448	-2.748739
H	3.458903	2.091603	-3.567757

H	2.491210	3.430574	-2.924737
N	-1.473059	-2.738081	-0.956628
C	-1.265176	-3.855276	-1.640739
C	-0.000039	-4.311275	-2.058689
H	-0.000043	-5.222508	-2.646211
C	1.265101	-3.855302	-1.640715
N	1.472994	-2.738110	-0.956604
C	-2.441297	-4.754808	-1.967499
H	-2.836802	-5.210838	-1.052560
H	-2.145661	-5.554513	-2.649733
H	-3.262137	-4.187901	-2.417828
C	2.441208	-4.754862	-1.967448
H	3.262075	-4.187975	-2.417754
H	2.145570	-5.554558	-2.649690
H	2.836676	-5.210904	-1.052498
C	-2.768129	-2.505166	-0.402690
C	-3.075402	-3.021879	0.865989
C	-4.314721	-2.722906	1.430837
H	-4.551843	-3.119432	2.417915
C	-5.253162	-1.933789	0.769163
C	-4.928774	-1.450391	-0.497429
H	-5.651772	-0.844560	-1.040496
C	-3.696808	-1.713049	-1.093749
C	-2.077290	-3.870996	1.611640
H	-1.771121	-4.750976	1.033243
H	-2.496250	-4.217233	2.561839
H	-1.166012	-3.302308	1.832188
C	-6.571234	-1.586234	1.414478
H	-6.548596	-0.566235	1.819589
H	-6.803961	-2.266940	2.239858
H	-7.395980	-1.632744	0.694450
C	-3.372175	-1.177538	-2.465673
H	-2.461270	-0.566639	-2.454311
H	-4.190256	-0.556589	-2.843502
H	-3.196471	-1.987380	-3.184735
C	2.768061	-2.505212	-0.402651
C	3.696764	-1.713124	-1.093711
C	4.928725	-1.450475	-0.497376
H	5.651742	-0.844668	-1.040444
C	5.253084	-1.933853	0.769232
C	4.314620	-2.722942	1.430905
H	4.551719	-3.119453	2.417995
C	3.075305	-3.021907	0.866041
C	3.372161	-1.177629	-2.465649
H	3.196450	-1.987480	-3.184700
H	4.190259	-0.556703	-2.843477
H	2.461268	-0.566712	-2.454308
C	6.571151	-1.586306	1.414560
H	7.395914	-1.632887	0.694557
H	6.803832	-2.266970	2.239987
H	6.548537	-0.566280	1.819608
C	2.077169	-3.871000	1.611688
H	1.165891	-3.302300	1.832206
H	2.496106	-4.217222	2.561903
H	1.771005	-4.750988	1.033302
C	-0.000019	-0.148789	1.301052
C	1.193985	-0.366426	2.026645
H	2.160181	-0.229114	1.534092
C	1.204319	-0.762474	3.364533
H	2.150523	-0.922575	3.877902

C	-0.000041	-0.960996	4.035522
H	-0.000049	-1.273052	5.077843
C	-1.204390	-0.762485	3.364510
H	-2.150601	-0.922596	3.877861
C	-1.194035	-0.366433	2.026624
H	-2.160223	-0.229122	1.534056

1a.log

SCF (wB97x) = -2008.24979542
E(SCF)+ZPE(0 K)= -2007.303868
H(298 K)= -2007.244075
G(298 K)= -2007.403947
Lowest Frequency = 10.4407 cm^{-1}

C	3.611986	1.974324	0.468024
C	2.511125	2.328901	1.262488
C	2.529548	2.085436	2.646706
C	3.665192	1.514003	3.217809
C	4.780237	1.172649	2.453124
C	4.733096	1.415850	1.082846
N	1.325563	2.843411	0.654516
C	1.148037	4.153759	0.557554
C	2.235464	5.084052	1.057127
C	1.330999	2.423597	3.497425
C	5.985797	0.523978	3.087174
C	3.577720	2.161169	-1.027772
Mg	0.000893	1.414962	0.002806
N	-1.321125	2.846821	-0.646980
C	-2.502921	2.335042	-1.264461
C	-3.607761	1.973570	-0.478747
C	-4.724184	1.416251	-1.103201
C	-4.762966	1.181753	-2.475247
C	-3.644488	1.530591	-3.231499
C	-2.513198	2.100465	-2.650356
C	-3.583502	2.151967	1.018341
C	-5.963259	0.534125	-3.120235
C	-1.310490	2.446224	-3.492127
C	-1.143822	4.156680	-0.543104
C	0.001574	4.762742	0.009868
C	-2.230006	5.089443	-1.040742
Mg	-0.006025	-1.415807	-0.001593
N	-1.331732	-2.844668	0.647125
C	-2.512226	-2.329939	1.264666
C	-2.522144	-2.095918	2.650612
C	-3.651912	-1.522911	3.231715
C	-4.769133	-1.170458	2.475346
C	-4.730771	-1.404654	1.103196
C	-3.615885	-1.965033	0.478817
C	-1.320720	-2.445666	3.492566
C	-5.967669	-0.519345	3.120089
C	-3.591817	-2.143243	-1.018298
N	1.314505	-2.847602	-0.654793
C	2.500880	-2.335697	-1.263430
C	3.601810	-1.979388	-0.467979
C	4.720182	-1.416074	-1.080755
C	4.767850	-1.172701	-2.452017
C	3.652265	-1.509938	-3.215849
C	2.517804	-2.087284	-2.645725
C	3.565510	-2.161957	1.028356

C	5.996875	-0.571675	-3.088265
C	1.316893	-2.417780	-3.496128
C	1.133366	-4.157505	-0.559151
C	-0.014441	-4.763794	-0.011282
C	-1.158048	-4.154940	0.542350
C	-2.246744	-5.085012	1.039522
C	2.217875	-5.090178	-1.060543
H	2.411365	-4.924849	-2.126061
H	1.942798	-6.136408	-0.912391
H	3.160536	-4.896298	-0.536565
H	-0.017607	-5.848082	-0.015361
H	-2.436733	-4.926558	2.106711
H	-1.978033	-6.131678	0.883019
H	-3.189610	-4.881925	0.519447
H	5.576139	-1.149751	-0.461137
H	3.660614	-1.314922	-4.287927
H	4.558257	-2.003116	1.462186
H	3.217130	-3.160603	1.314561
H	2.886649	-1.433095	1.493361
H	6.466391	0.166742	-2.428261
H	5.753880	-0.073964	-4.032756
H	6.749068	-1.340391	-3.304373
H	1.505024	-2.175855	-4.546712
H	0.433662	-1.852076	-3.171467
H	1.048200	-3.478952	-3.434075
H	-3.657805	-1.345466	4.306977
H	-5.592459	-1.138151	0.491726
H	-1.061384	-3.508433	3.418847
H	-1.502319	-2.212456	4.546256
H	-0.434075	-1.884451	3.169577
H	-5.825251	0.565257	3.212244
H	-6.142930	-0.911059	4.127713
H	-6.875800	-0.682907	2.530484
H	-4.587203	-1.979194	-1.444088
H	-3.249643	-3.142394	-1.310211
H	-2.913600	-1.415795	-1.486381
H	-2.420292	4.931086	-2.107893
H	-1.958527	6.135451	-0.884624
H	-3.173461	4.889053	-0.520694
H	0.001407	5.847034	0.013096
H	2.430051	4.918947	2.122471
H	1.962697	6.130846	0.908736
H	3.176996	4.887700	0.532071
H	-5.586734	1.152409	-0.491800
H	-3.650642	1.352734	-4.306697
H	-4.579519	1.991192	1.443909
H	-3.238177	3.150045	1.310201
H	-2.907763	1.422380	1.486679
H	-5.821034	-0.549930	-3.218831
H	-6.141368	0.931387	-4.125199
H	-6.869739	0.694423	-2.527212
H	-1.492548	2.213188	-4.545778
H	-0.425656	1.882400	-3.168705
H	-1.047867	3.508200	-3.418735
H	3.677736	1.329213	4.291780
H	5.593265	1.158513	0.465218
H	1.065613	3.485380	3.431673
H	1.519672	2.184888	4.548641
H	0.445610	1.859578	3.175876
H	5.847246	-0.561141	3.179165

H	6.168268	0.914865	4.093850
H	6.888625	0.690843	2.490383
H	4.567862	1.993185	-1.463764
H	3.238916	3.163945	-1.311337
H	2.891344	1.440527	-1.494305

1a-H2.log

SCF (wB97x) = -2009.47274887
E(SCF)+ZPE(0 K)= -2008.512618
H(298 K)= -2008.452864
G(298 K)= -2008.608893
Lowest Frequency = 13.0142 cm^{-1}

C	3.707642	2.004080	0.061899
C	2.668238	2.296040	0.956746
C	2.826284	2.059853	2.333278
C	4.043348	1.561434	2.794433
C	5.104194	1.294631	1.929298
C	4.916214	1.528102	0.569638
N	1.415951	2.777557	0.464320
C	1.210925	4.086327	0.390823
C	2.332233	5.028870	0.780564
C	1.696479	2.339207	3.292165
C	6.403608	0.729560	2.447169
C	3.518201	2.178686	-1.424255
Mg	0.002133	1.392614	-0.006122
N	-1.410010	2.776195	-0.485820
C	-2.667986	2.291631	-0.960235
C	-3.700395	2.018644	-0.052031
C	-4.914273	1.535711	-0.541093
C	-5.113944	1.278804	-1.894353
C	-4.059605	1.527988	-2.773263
C	-2.837978	2.031529	-2.331409
C	-3.498672	2.222181	1.428803
C	-6.418636	0.709497	-2.394167
C	-1.715301	2.290834	-3.304207
C	-1.199539	4.084963	-0.433218
C	0.007582	4.688114	-0.027627
C	-2.318519	5.025809	-0.833516
Mg	0.002121	-1.392613	0.006137
N	-1.410033	-2.776185	0.485830
C	-2.668008	-2.291613	0.960238
C	-2.838006	-2.031508	2.331410
C	-4.059634	-1.527963	2.773257
C	-5.113968	-1.278778	1.894342
C	-4.914291	-1.535688	0.541084
C	-3.700412	-2.018625	0.052028
C	-1.715334	-2.290816	3.304214
C	-6.418661	-0.709467	2.394149
C	-3.498683	-2.222168	-1.428804
N	1.415927	-2.777566	-0.464314
C	2.668215	-2.296057	-0.956745
C	3.707624	-2.004103	-0.061903
C	4.916196	-1.528128	-0.569647
C	5.104169	-1.294656	-1.929307
C	4.043319	-1.561454	-2.794438
C	2.826255	-2.059869	-2.333278
C	3.518190	-2.178717	1.424251
C	6.403581	-0.729586	-2.447185

C	1.696444	-2.339216	-3.292160
C	1.210893	-4.086335	-0.390815
C	0.007547	-4.688114	0.027639
C	-1.199570	-4.084954	0.433229
C	-2.318557	-5.025793	0.833525
C	2.332193	-5.028886	-0.780562
H	2.627195	-4.869061	-1.823447
H	2.033935	-6.071727	-0.657031
H	3.222544	-4.841795	-0.170290
H	0.010034	-5.772106	0.036769
H	-2.620897	-4.848173	1.871404
H	-2.014555	-6.069244	0.730954
H	-3.205940	-4.854378	0.214371
H	5.729619	-1.320598	0.125153
H	4.166979	-1.381620	-3.862188
H	4.459543	-2.010858	1.957438
H	3.150322	-3.178956	1.680327
H	2.787850	-1.456156	1.813143
H	6.347551	0.362802	-2.547281
H	6.651913	-1.132866	-3.434663
H	7.234419	-0.954687	-1.770192
H	1.997117	-2.118327	-4.321076
H	0.819862	-1.723962	-3.053603
H	1.372815	-3.386309	-3.250425
H	-4.192476	-1.328796	3.836546
H	-5.721635	-1.340422	-0.164180
H	-1.387318	-3.337143	3.281762
H	-2.025802	-2.054970	4.326887
H	-0.839176	-1.675824	3.063523
H	-6.331272	0.367773	2.589147
H	-6.731481	-1.183053	3.331083
H	-7.220356	-0.847737	1.661037
H	-4.428470	-2.035207	-1.975761
H	-3.158168	-3.237201	-1.664561
H	-2.741875	-1.529274	-1.820455
H	-2.620851	4.848197	-1.871398
H	-2.014514	6.069258	-0.730936
H	-3.205907	4.854393	-0.214371
H	0.010076	5.772107	-0.036755
H	2.627247	4.869037	1.823444
H	2.033979	6.071714	0.657044
H	3.222576	4.841780	0.170280
H	-5.721620	1.340445	0.164166
H	-4.192442	1.328823	-3.836553
H	-4.428462	2.035222	1.975754
H	-3.158154	3.237212	1.664564
H	-2.741870	1.529282	1.820456
H	-6.331237	-0.367735	-2.589208
H	-6.731472	1.183115	-3.331080
H	-7.220324	0.847730	-1.661042
H	-2.025763	2.054989	-4.326882
H	-0.839145	1.675841	-3.063510
H	-1.387282	3.337160	-3.281753
H	4.167012	1.381601	3.862183
H	5.729633	1.320567	-0.125166
H	1.372850	3.386300	3.250426
H	1.997159	2.118324	4.321081
H	0.819896	1.723951	3.053617
H	6.347606	-0.362838	2.547182
H	6.651901	1.132774	3.434683

H	7.234457	0.954734	1.770215
H	4.459558	2.010850	-1.957443
H	3.150305	3.178913	-1.680334
H	2.787881	1.456102	-1.813143
H	0.001568	0.005974	1.283701
H	0.001564	-0.005973	-1.283685

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