Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Synthesis, Structure and Gas-Phase Reactivity of the Mixed Silver Hydride Borohydride Nanocluster $[Ag_3(\mu_3\text{-}H)(\mu_3\text{-}BH_4)L^{Ph}_3]BF_4$ (L^{Ph} = bis(diphenylphosphino)methane).

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Contents

Complete citation for reference 46

Gaussian 09, revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Description of conversion of NCE to voltage for ERCID experiments.

The NCE was converted to an amplitude of the resonance excitation RF voltage (tick amp) (eq. 13). The tick amp slope and tick amp intercept are extracted from the normalised collision energy calibration file of the most recent calibration.

Amplitude (V)	=	(NCE)% ÷ 30%((parent mass)(tick amp slope) + tick amp intercept)	(eq. 13)

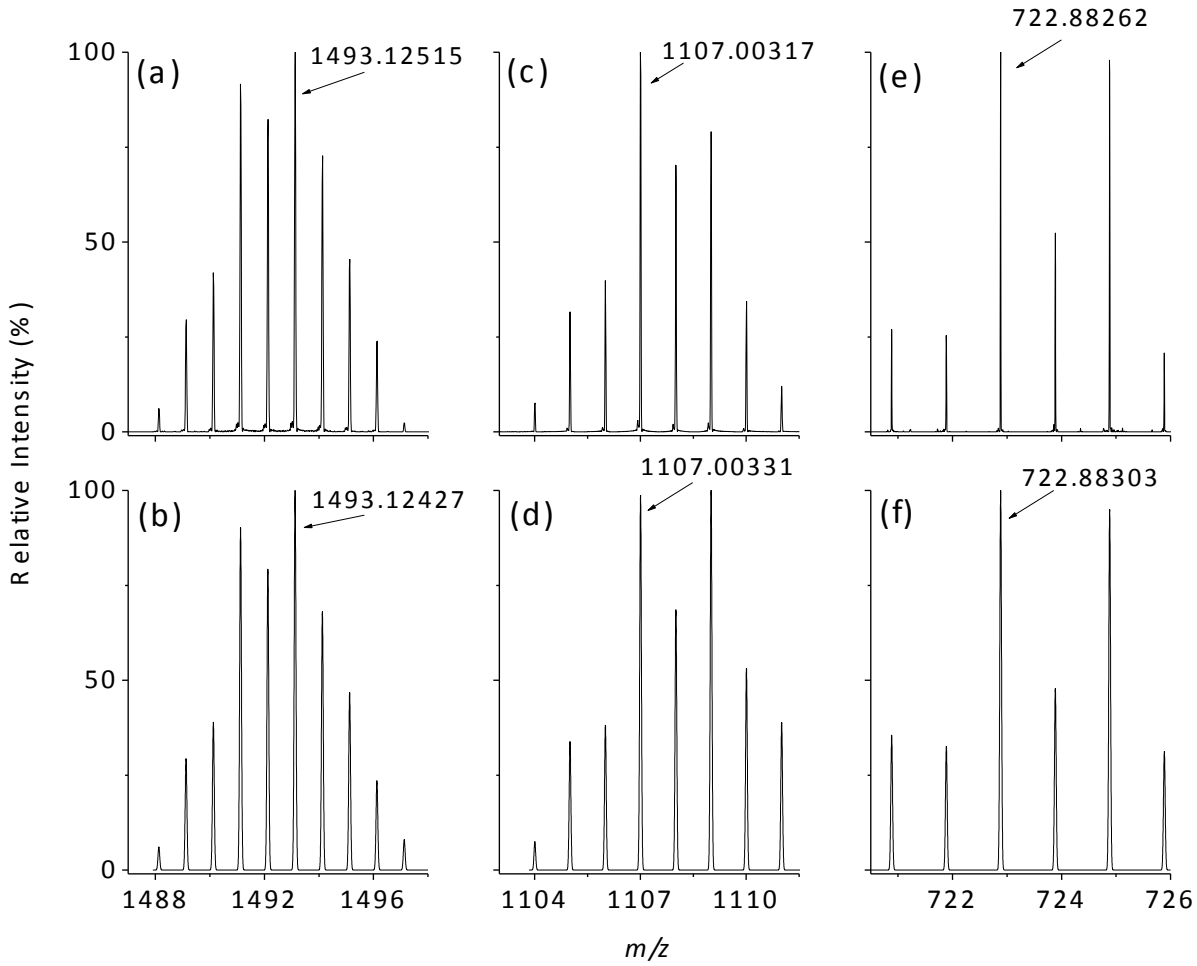

Figure S1: LTQ/FTICR high resolution ESI/MS of hydride/borohydride containing trinuclear silver(I) clusters. Comparison of measured (top panel) vs. simulated isotope ratios (bottom panel) and accurate mass determination for: (a) measured HR FT-ICR MS of $[Ag_3(H)(BH_4)L_3]^+$, 0.6 ppm error; (b) simulated isotope distribution of $[Ag_3(H)(BH_4)L_3]^+$; (c) measured HR FT-ICR MS of $[Ag_3(H)(BH_4)L_2]^+$, 0.1 ppm error; (d) simulated isotope distribution of $[Ag_3(H)(BH_4)L_2]^+$; (e) measured HR FT-ICR MS of $[Ag_3(H)(BH_4)L]^+$, 0.6 ppm error; (f) simulated isotope distribution of $[Ag_3(H)(BH_4)L]^+$. L = dppm = bis(diphenylphosphino)methane. The most intense isotope peak is represented by the *m/z* value.

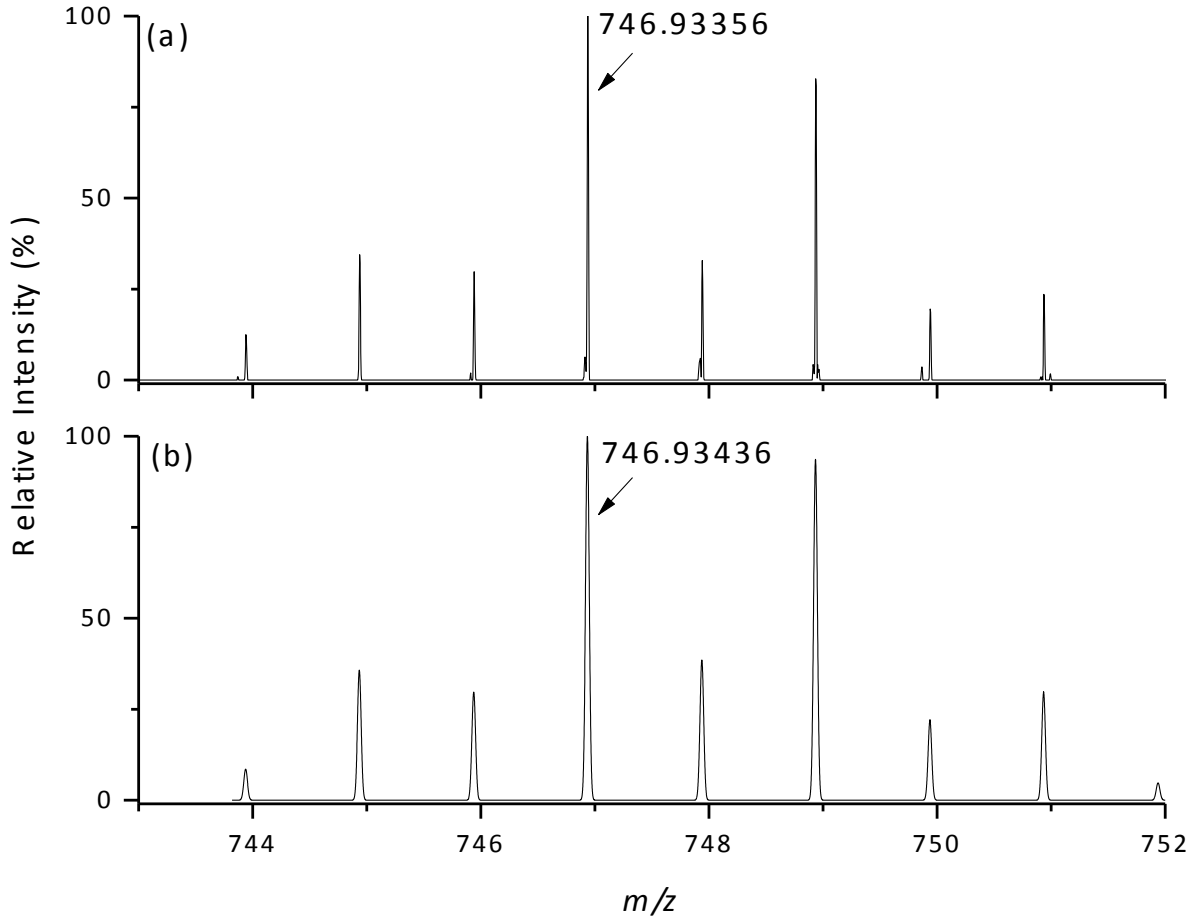

Figure S2: LTQ/FTICR high resolution ESI/MS of hydride/borohydride containing trinuclear silver(I) clusters. Comparison of measured (top panel) vs. simulated isotope ratios (bottom panel) and accurate mass determination for: (a) measured HR FT-ICR MS of $[Ag_3(H)(BH_4)L_3]^+$, 0.6 ppm error; (b) simulated isotope distribution of $[Ag_3(H)(BH_4)L_3]^+$. L = dmpm = bis(dimethylphosphino)methane. The most intense isotope peak is represented by the *m/z* value.

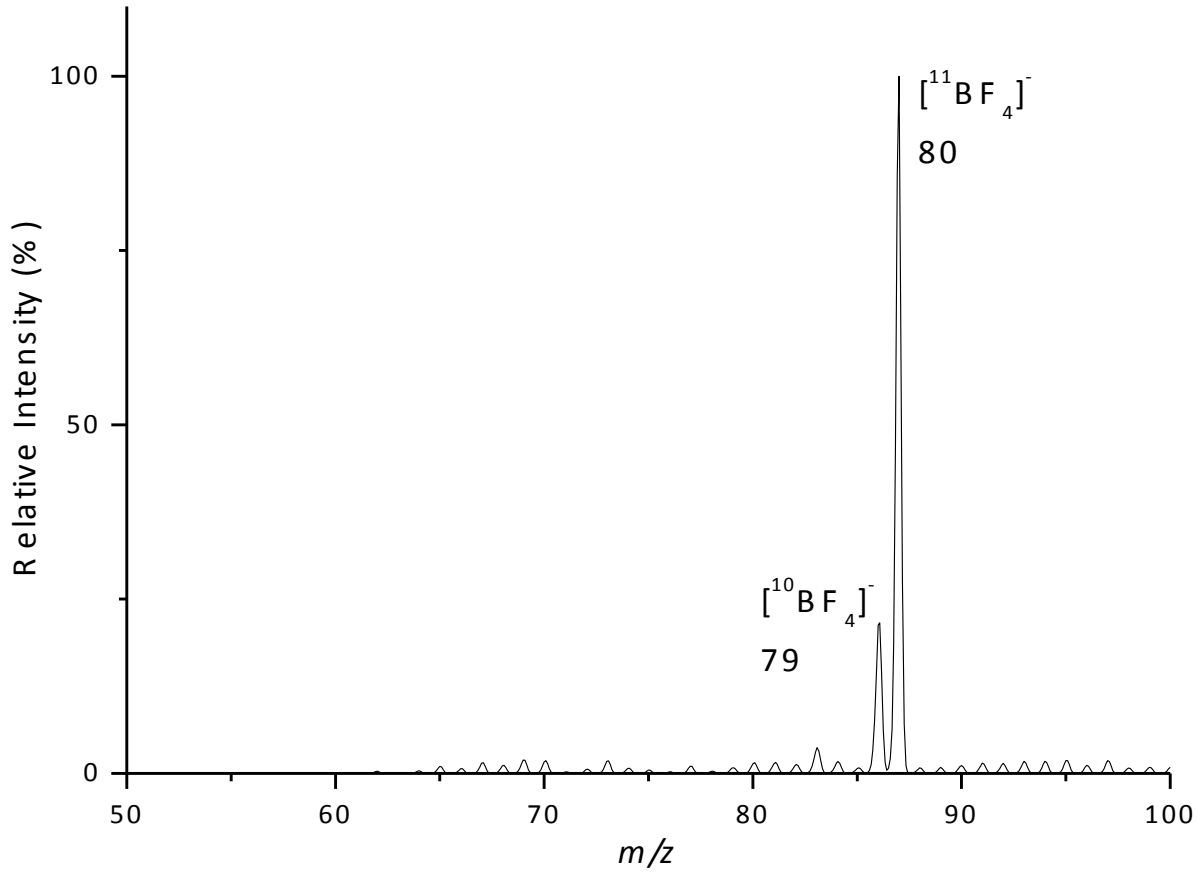

Figure S3: LTQ ESI/MS in the negative ion polarity mode of an acetonitrile solution of **1**. Solutions were diluted to ca. 50 μM in acetonitrile. The most intense isotope peak is represented by the *m/z* value.

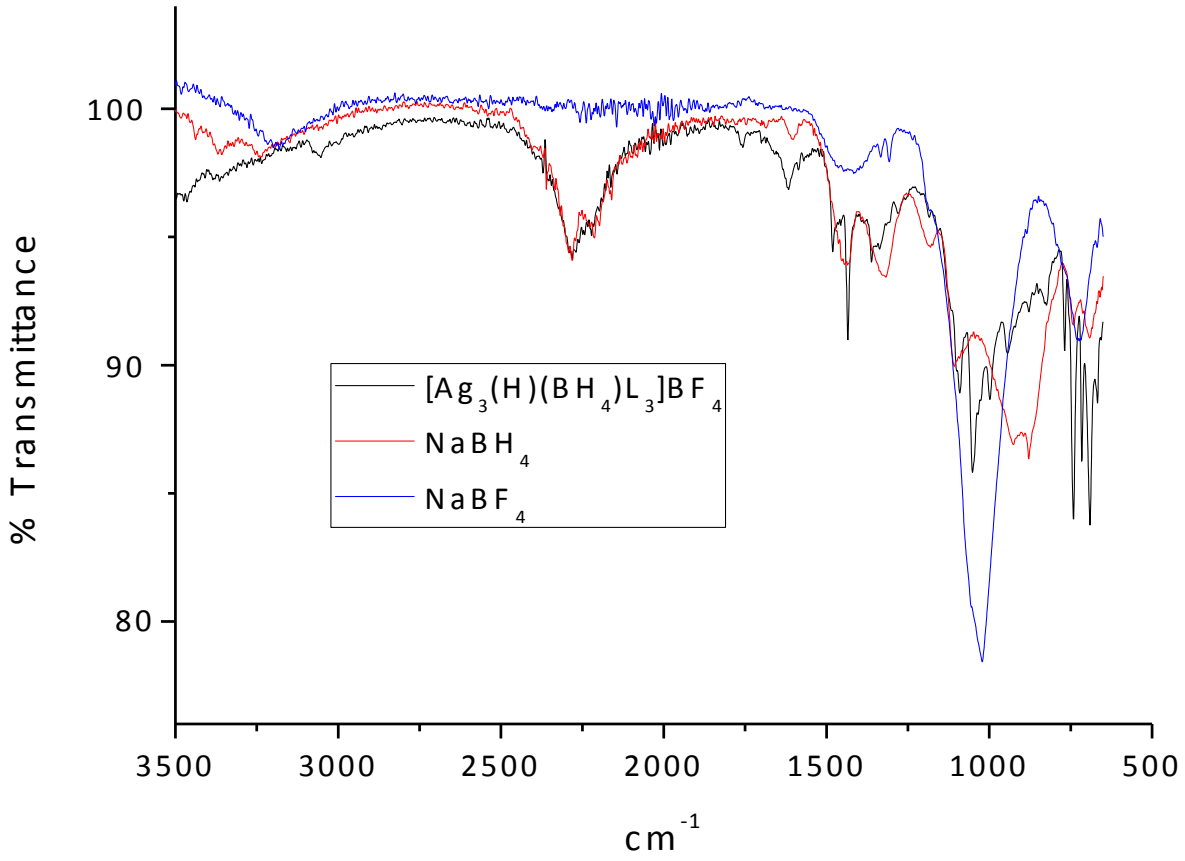

Figure S4: FT-IR spectra of: $[Ag_3(H)(BH_4)L_3]BF_4$ shown by the black line, $NaBH_4$ shown by the red line and $NaBF_4$ shown by the blue line. All spectra were collected from material as fine powders after mechanical grinding in a mortar and pestle and subsequently recorded using a Perkin-Elmer Spectrum one FTIR spectrometer operating in the diffuse reflectance mode. Each spectrum is an average of 32 scans.

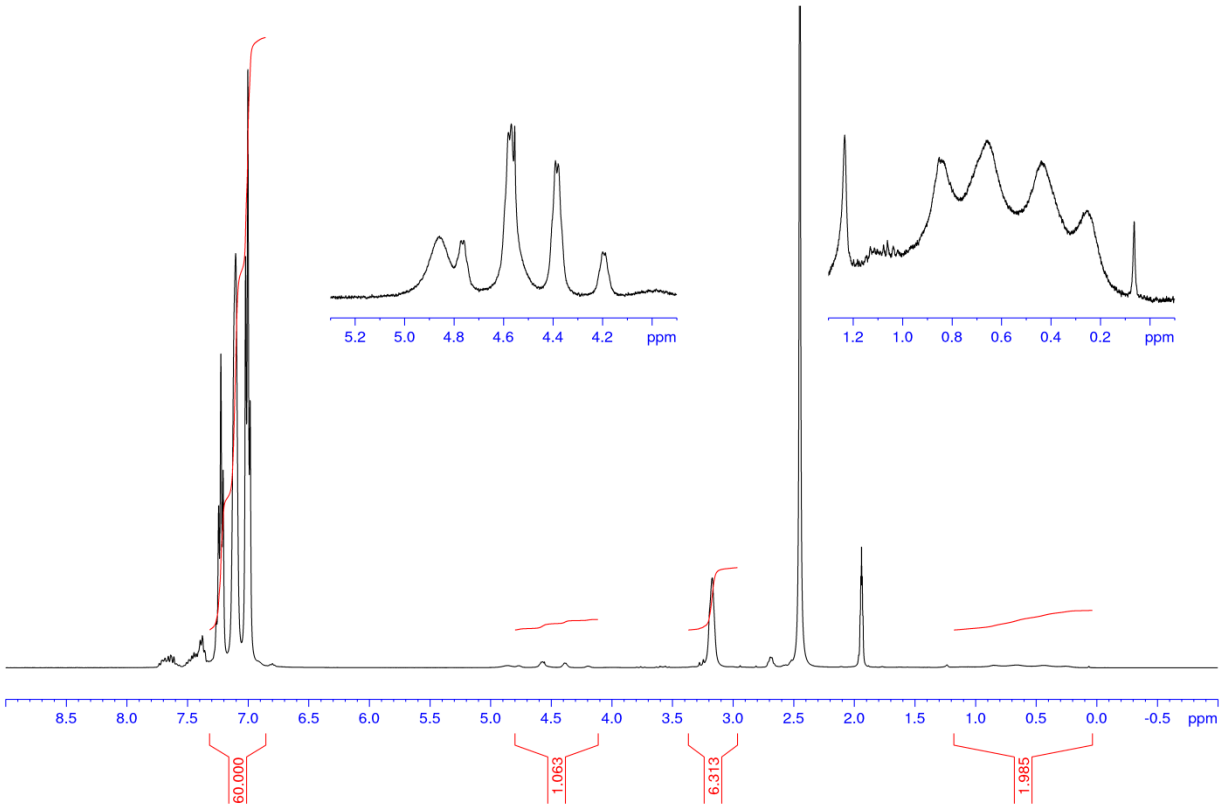

Figure S5: ^{1}H NMR spectrum of **1** (400.1 MHz, CD_3CN) at -15°C. Insets are the μ_3-H (5.3 to 3.9 ppm) and μ_3-BH_4 (1.3 to -0.1 ppm) signals.

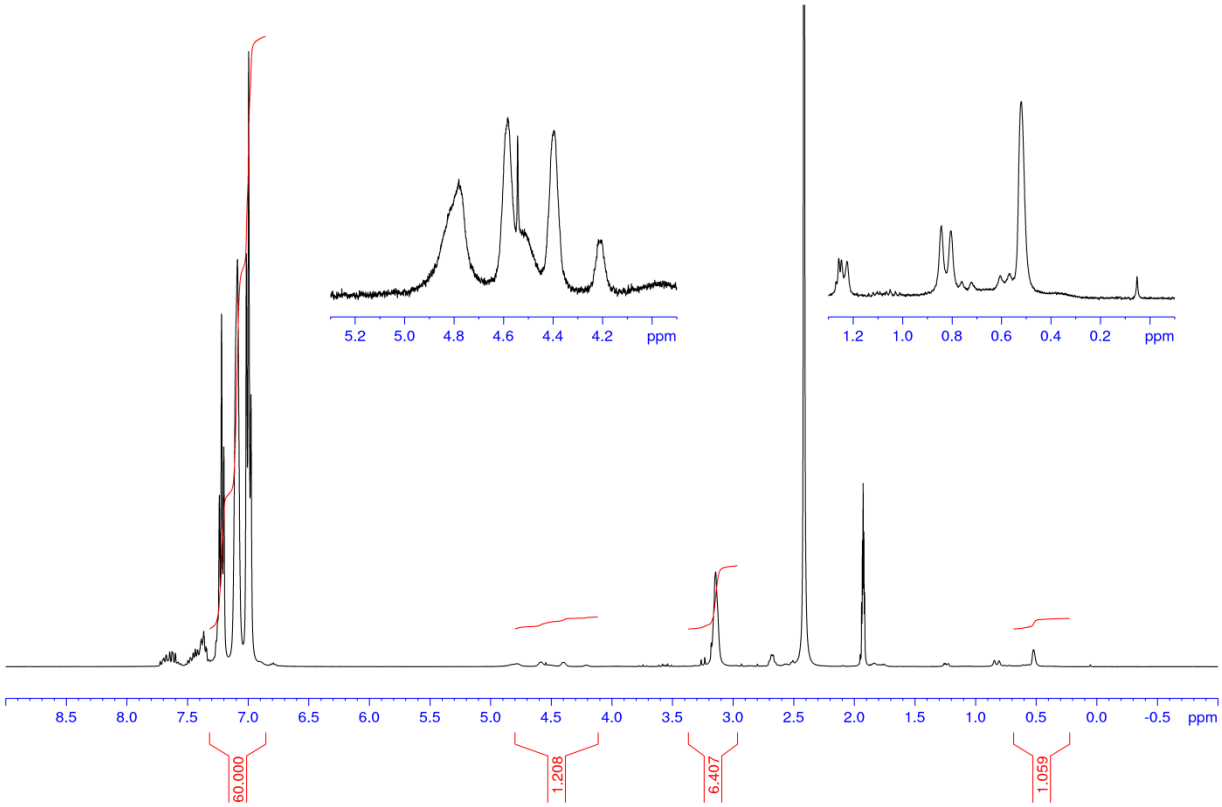

Figure S6: ^{11}B-decoupled ^{1}H NMR spectrum of **1** (400.1 MHz, CD_3CN) at -15°C. Insets are the μ_3-H (5.3 to 3.9 ppm) and μ_3-BH_4 (1.3 to -0.1 ppm) signals.

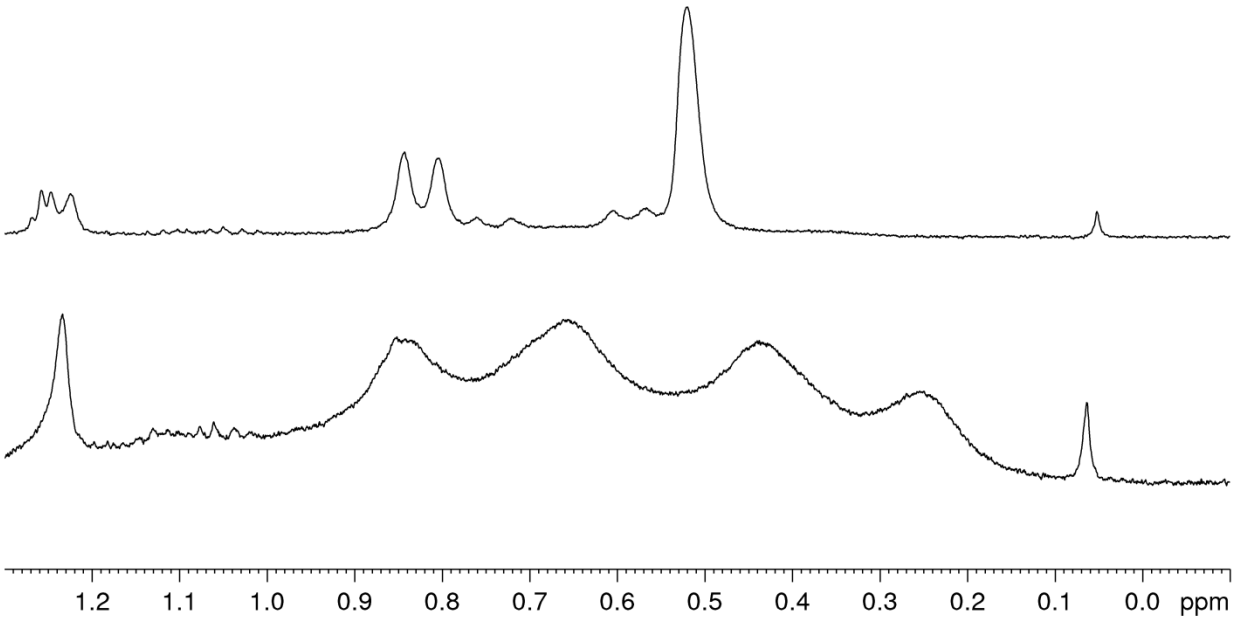

Figure S7: Overlay of the ^{11}B-decoupled ^{1}H (upper) and ^{1}H (lower) NMR spectra of **1** (400.1 MHz, CD_3CN) at -15°C of the μ_3-BH_4 (1.3 to -0.1 ppm) signals.

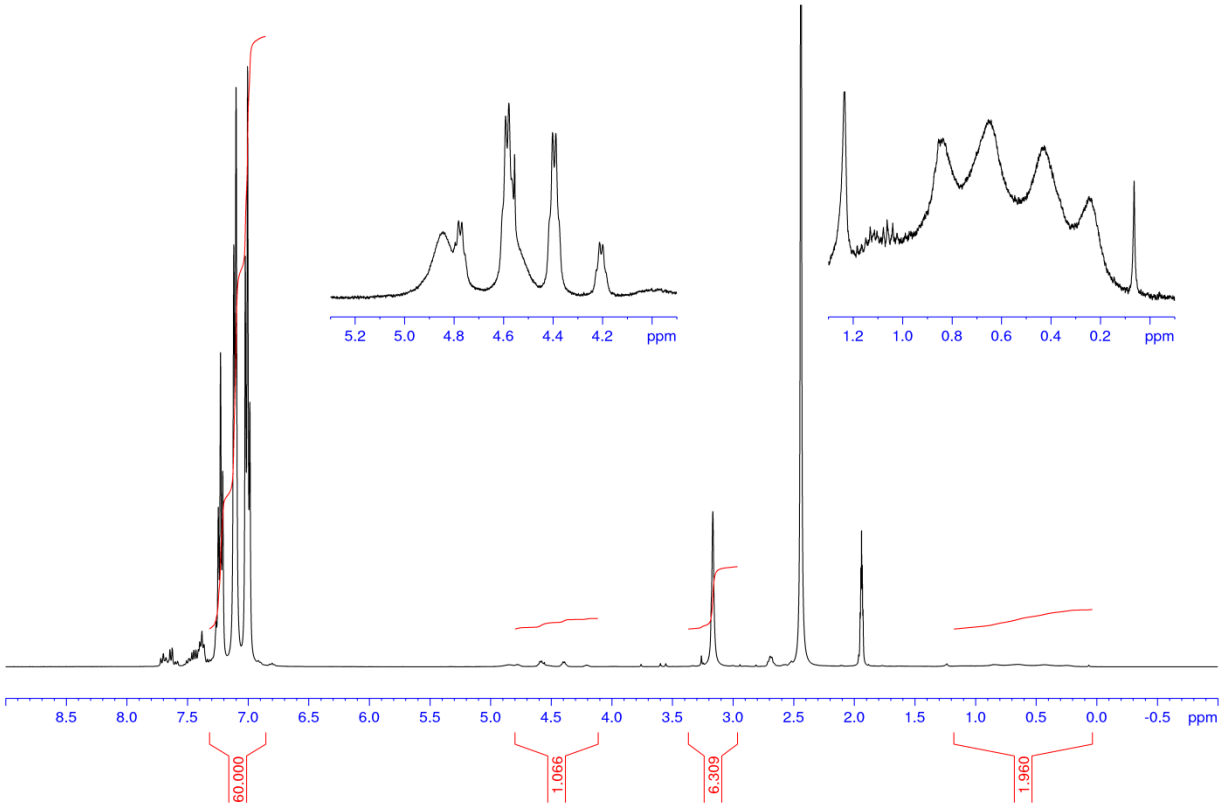

Figure S8: ^{31}P-decoupled ^{1}H NMR spectrum of **1** (400.1 MHz, CD_3CN) at -15°C. Insets are the μ_3-H (5.3 to 3.9 ppm) and μ_3-BH_4 (1.3 to -0.1 ppm) signals.

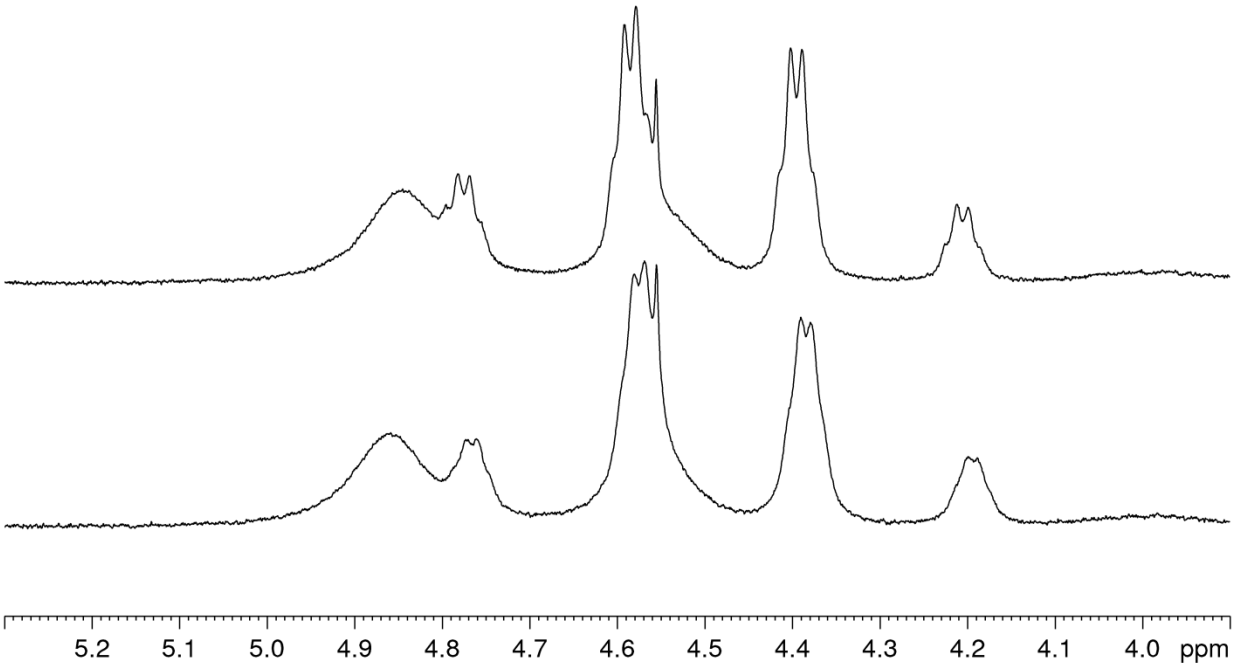

Figure S9: Overlay of the ^{31}P-decoupled ^{1}H (upper) and ^{1}H (lower) NMR spectra of **1** (400.1 MHz, CD_3CN) at -15°C of the μ_3-H (5.3 to 3.9 ppm) signals.

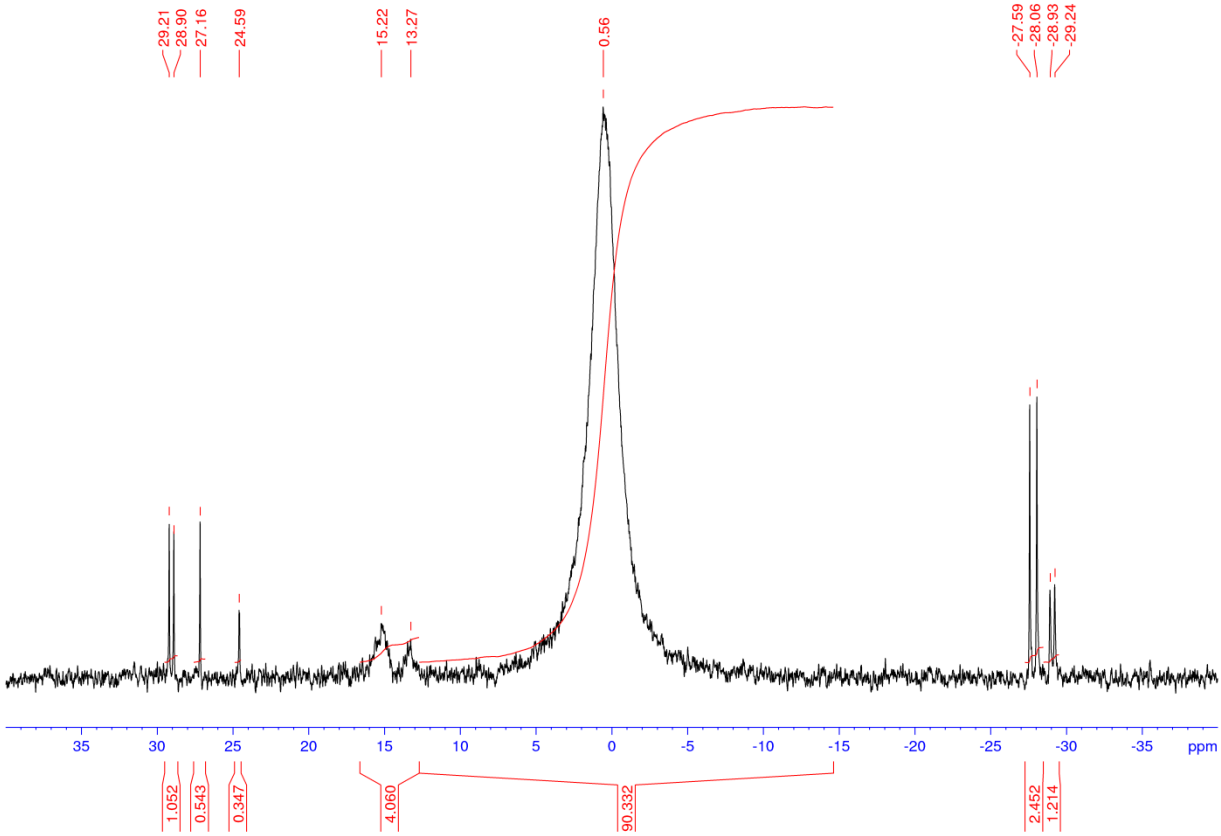

Figure S10: ^{1}H-decoupled ^{31}P NMR spectrum of **1** (162.0 MHz, CD_3CN) at -15°C.

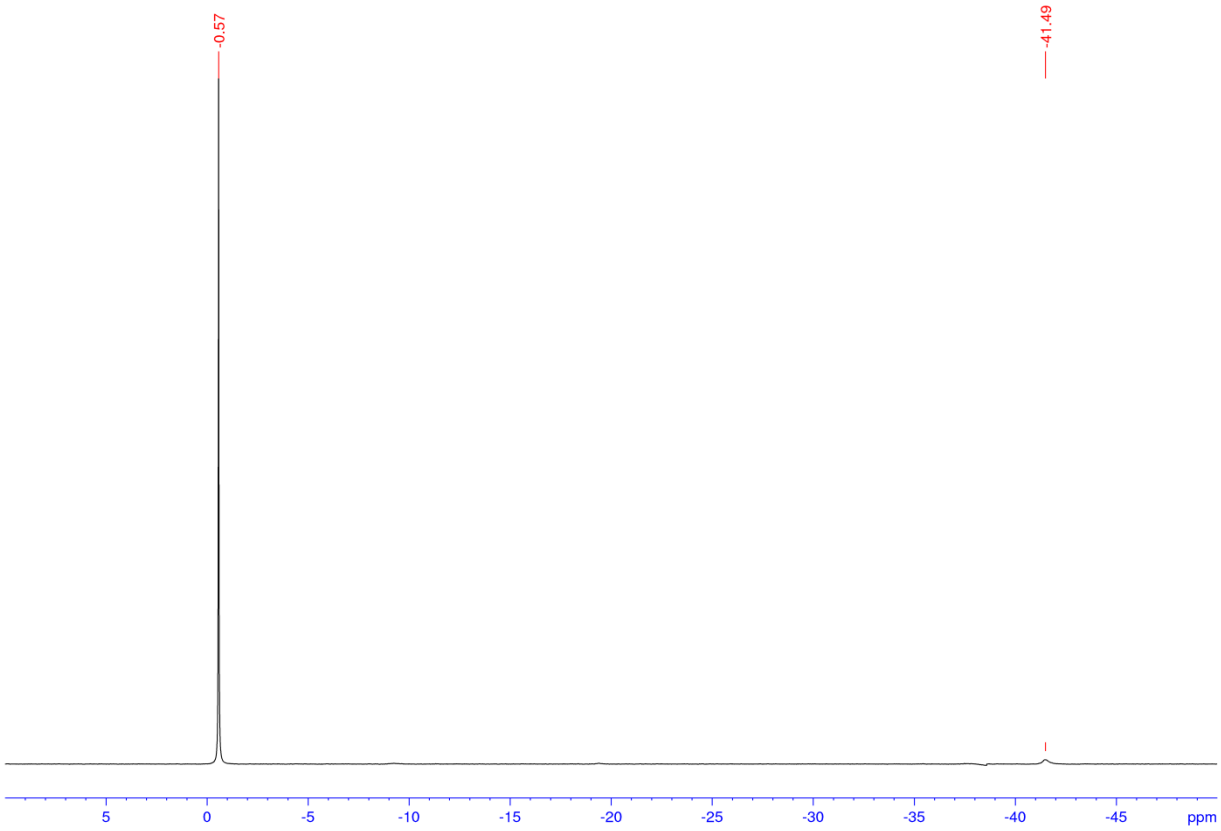

Figure S11: ^{1}H-decoupled ^{11}B NMR spectrum of **1** (128.4 MHz, CD_3CN) at -15°C.

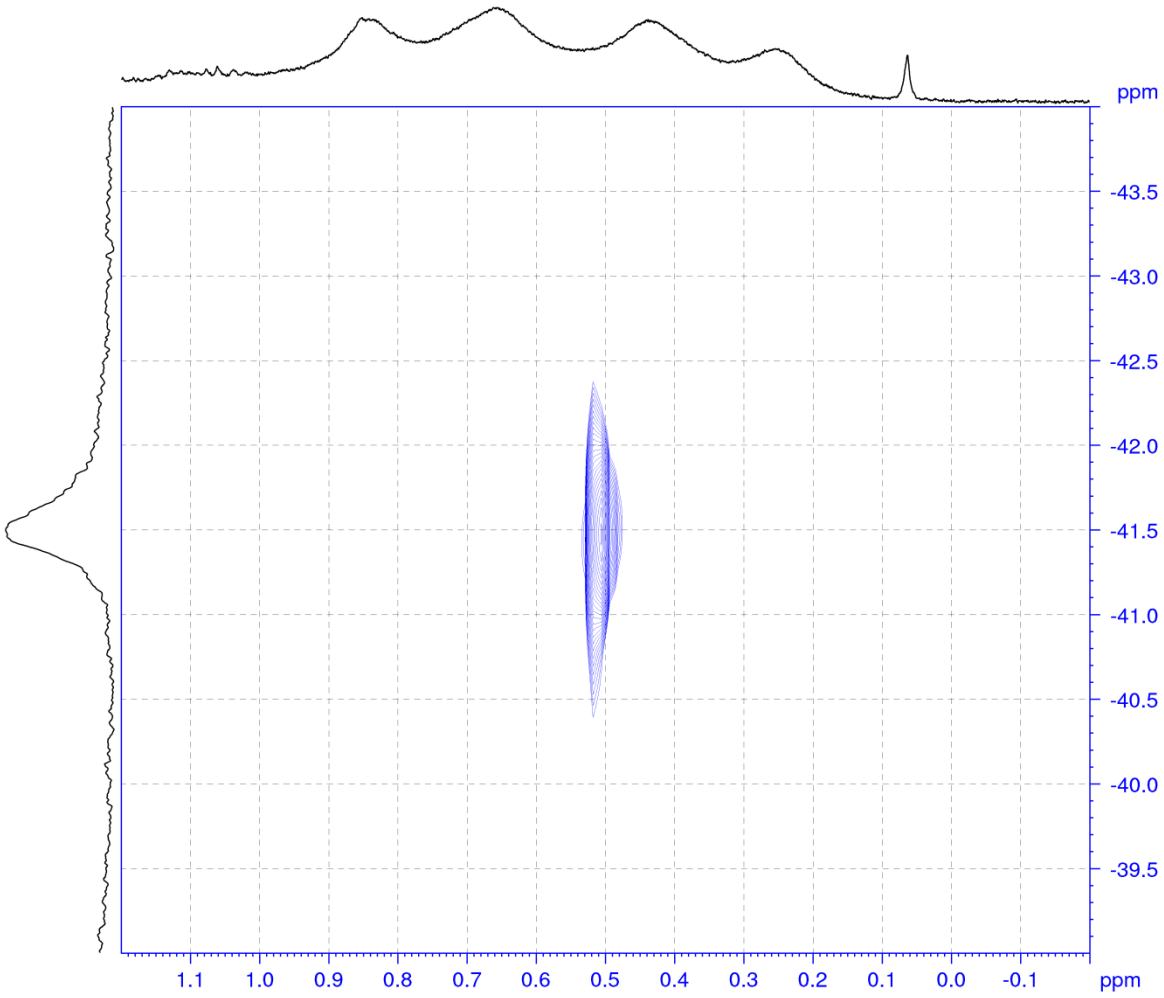

Figure S12: ^{1}H-^{11}B HSQC spectrum of **1** (400.1 MHz (^{1}H), 128.4 MHz (^{11}B), CD_3CN) at -15°C.

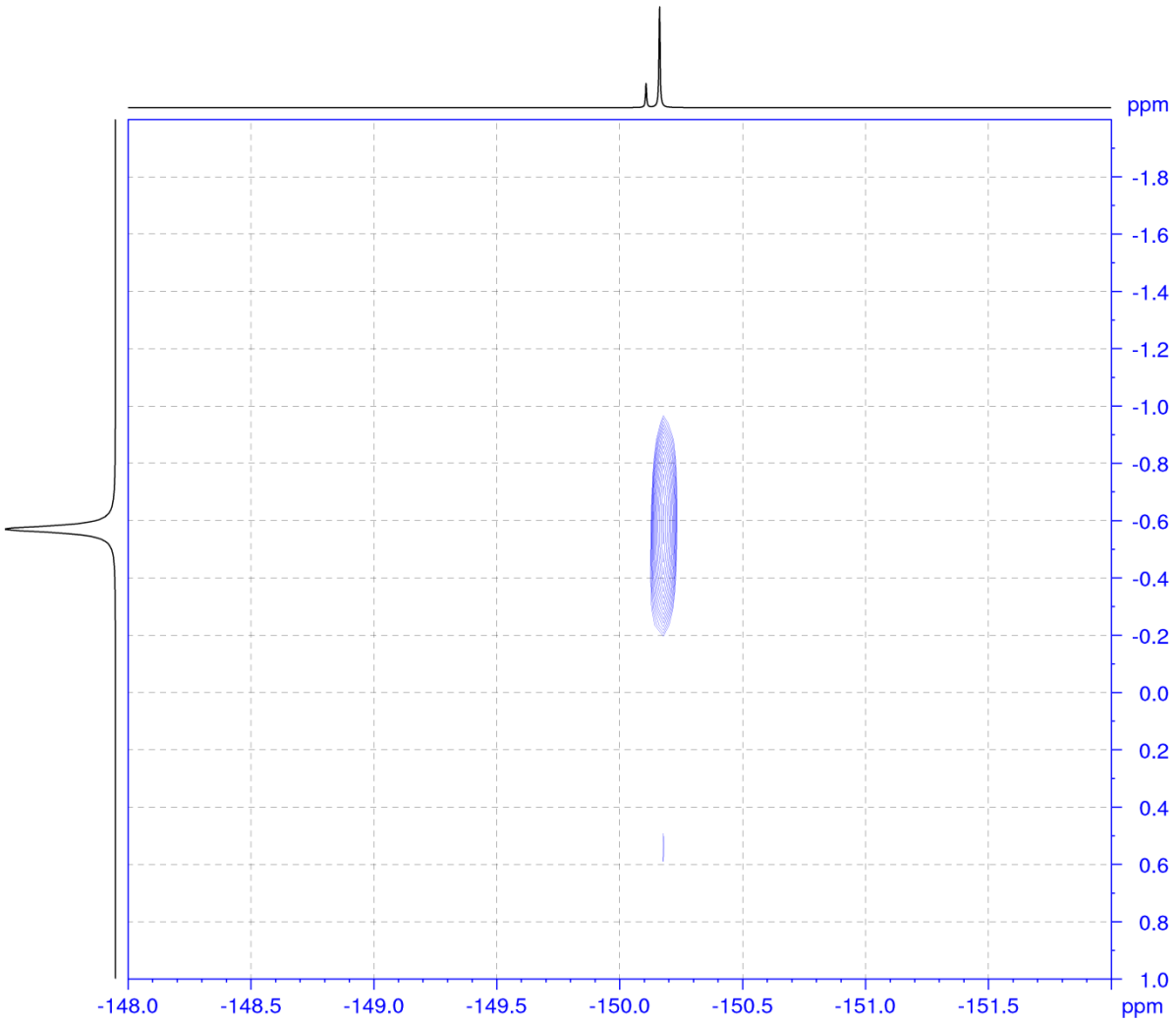

Figure S13: ^{19}F-^{11}B HSQC spectrum of **1** (376.5 MHz (^{19}F), 128.4 MHz (^{11}B), CD_3CN) at -15°C.

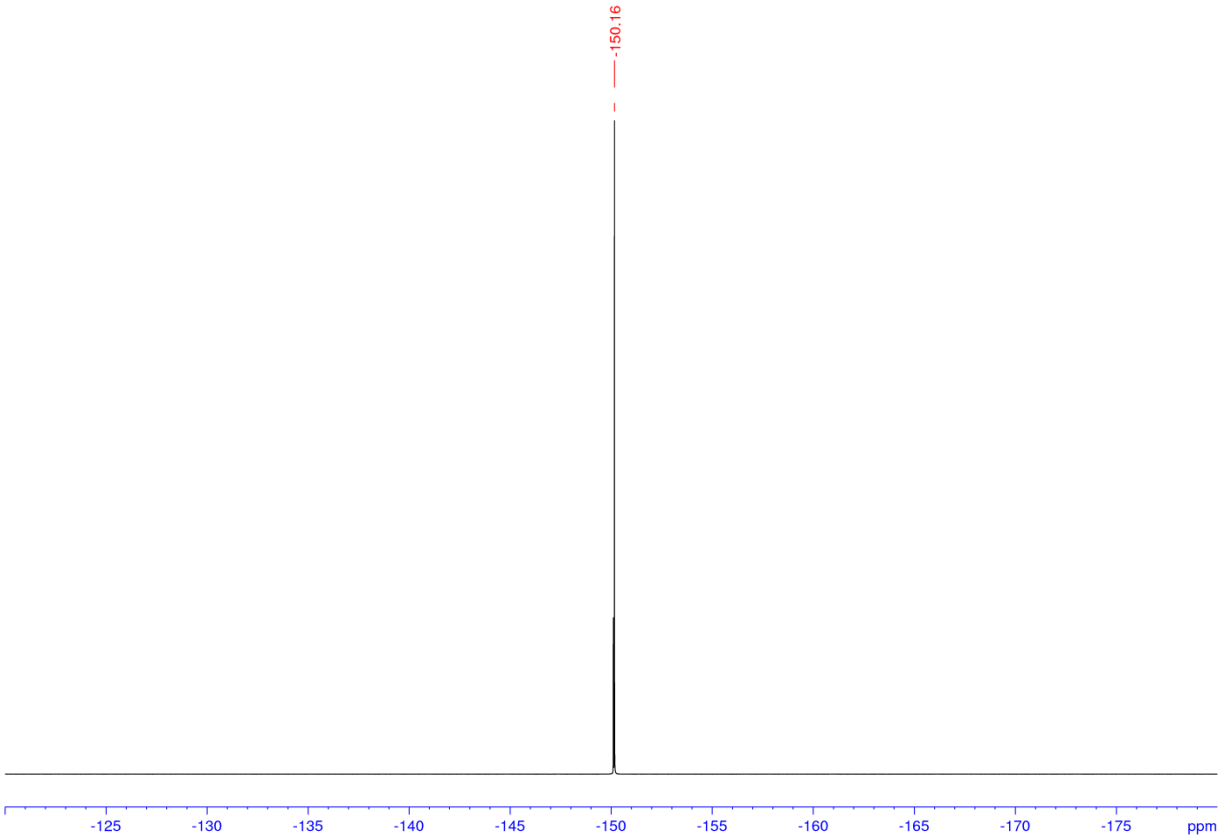

Figure S14: ^{1}H-decoupled ^{19}F NMR spectrum of **1** (376.5 MHz, CD_3CN) at -15°C.

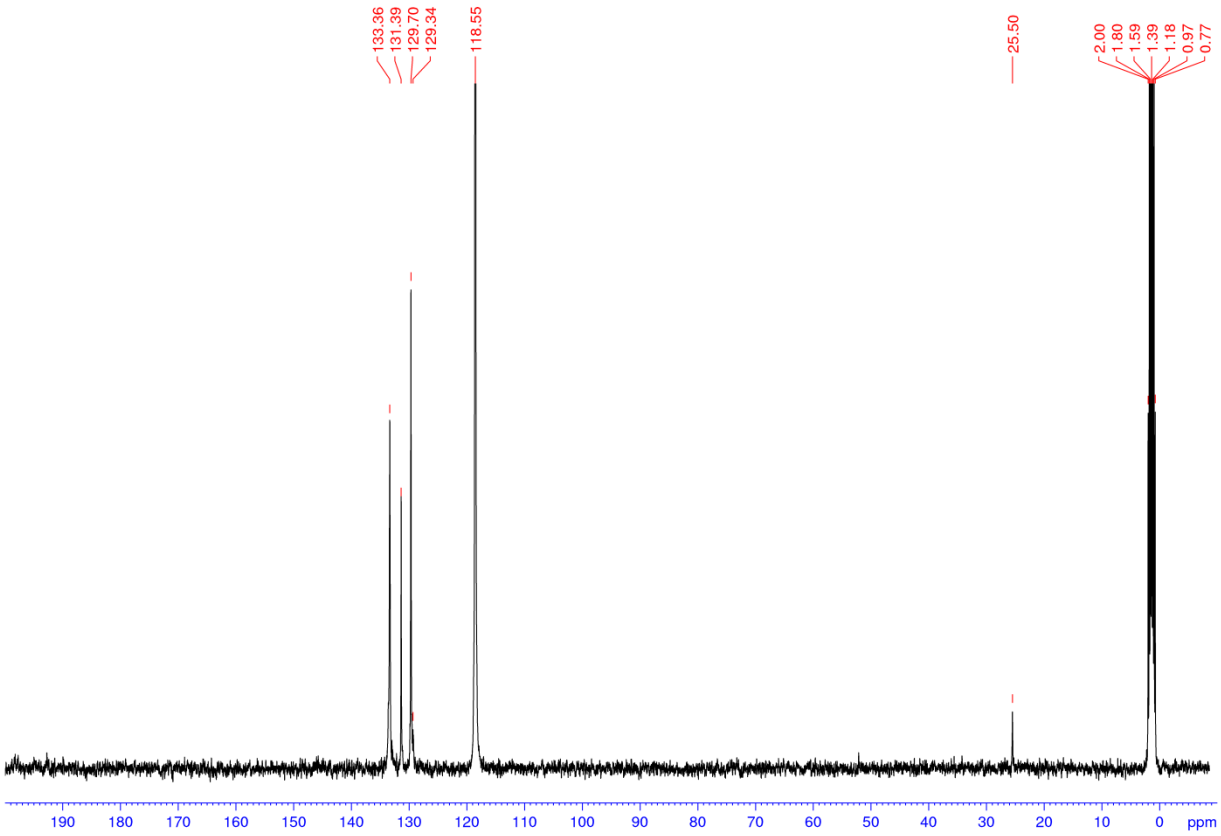

Figure S15: ^{1}H-decoupled ^{13}C NMR spectrum of **1** (100.6 MHz, CD_3CN) at -15°C.

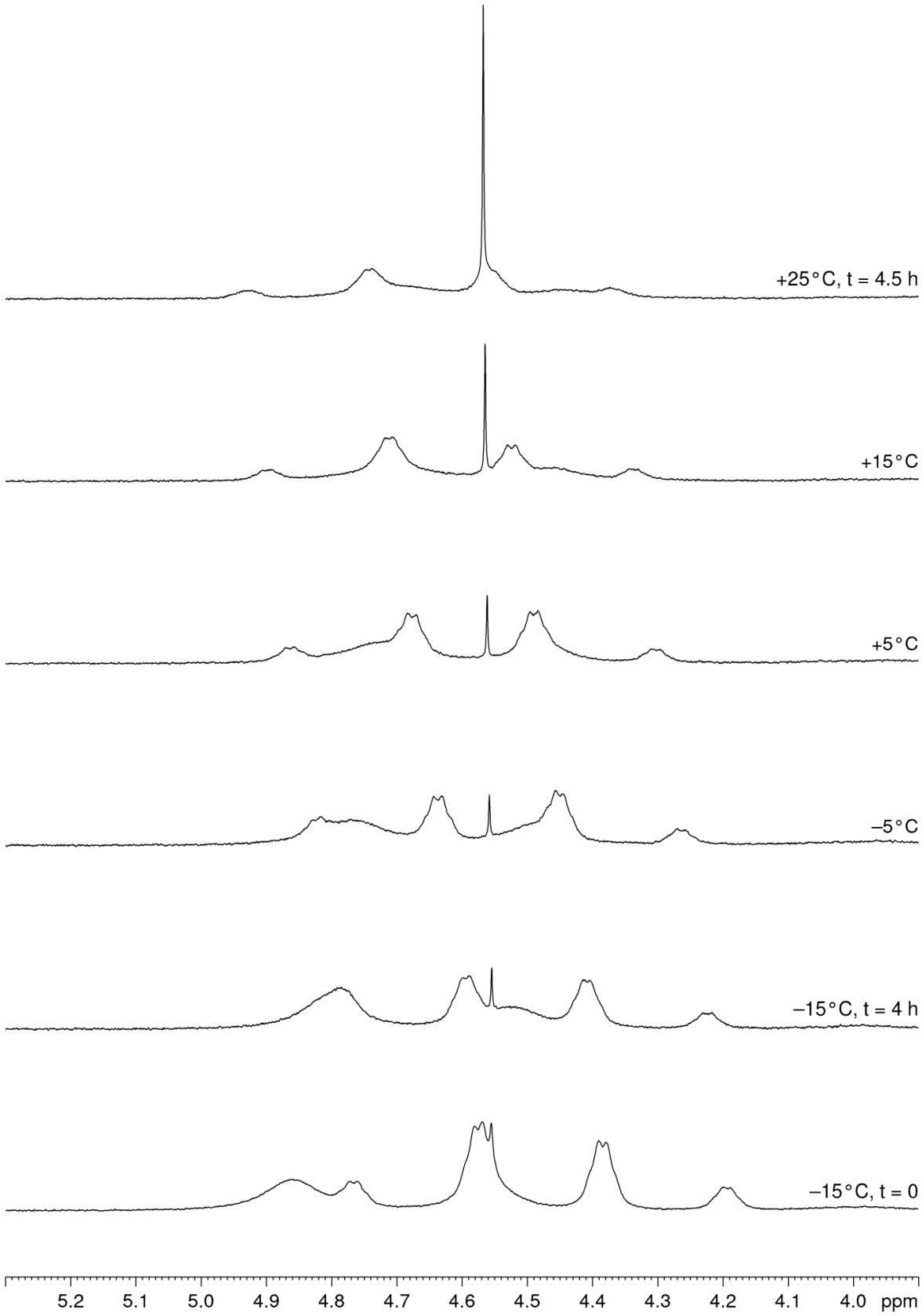

Figure S16: ^{1}H NMR spectrum of **1** (400.1 MHz, CD_3CN) recorded at temperatures from -15°C to +25°C; μ_3-H (5.3 to 3.9 ppm)and H_2 (4.56 ppm) signals.

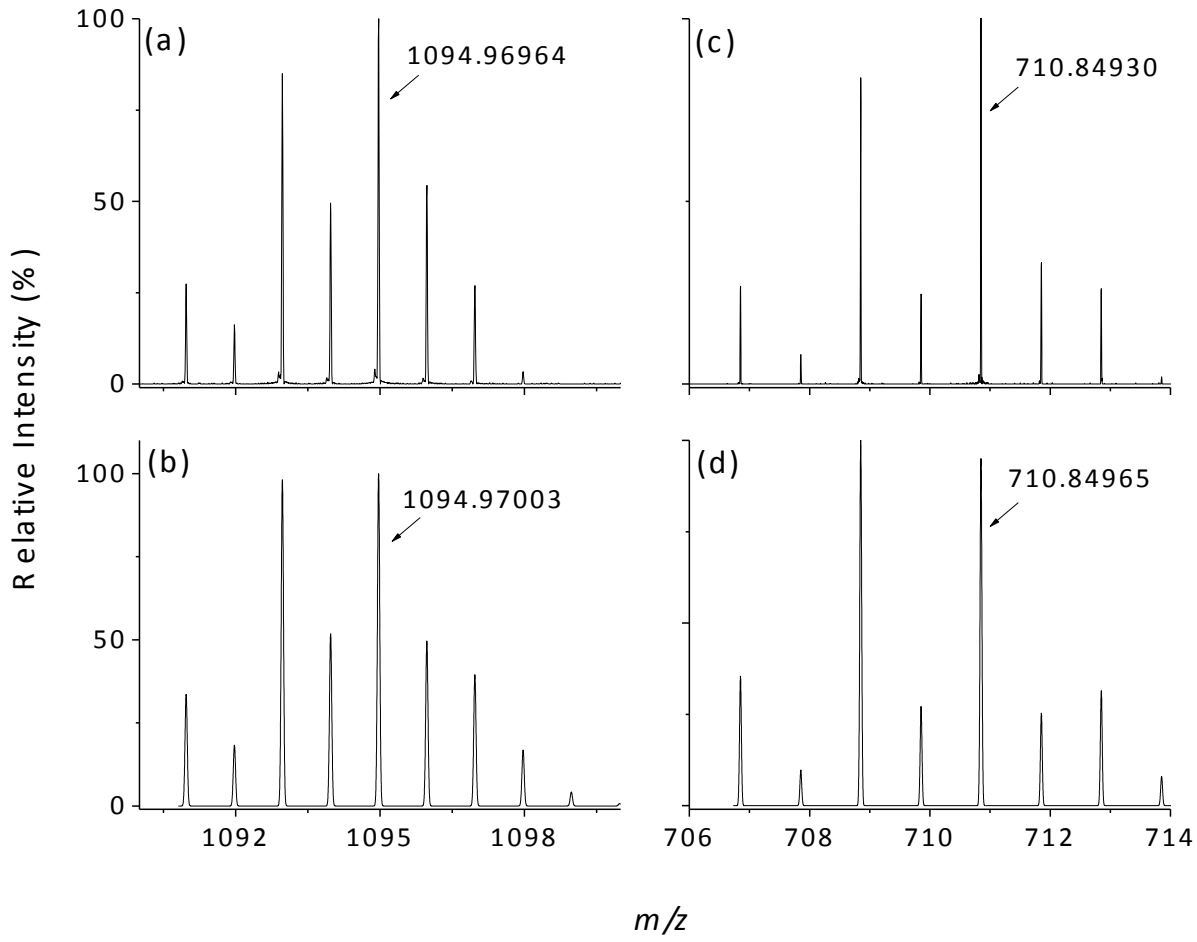

Figure S17: LTQ/FTICR high resolution ESI/MS of dihydride containing trinuclear silver(I) clusters. Comparison of measured (top panel) vs. simulated isotope ratios (bottom panel) and accurate mass determination for: (a) measured HR FT-ICR MS of $[Ag_3(H)_2L_2]^+$, 0.4 ppm error; (b) simulated isotope distribution of $[Ag_3(H)_2L_2]^+$; (c) measured HR FT-ICR MS of $[Ag_3(H)_2L]^+$, 0.5 ppm error; (d) simulated isotope distribution of $[Ag_3(H)_2L]^+$. L = dppm = bis(diphenylphosphino)methane. The most intense isotope peak is represented by the *m/z* value.

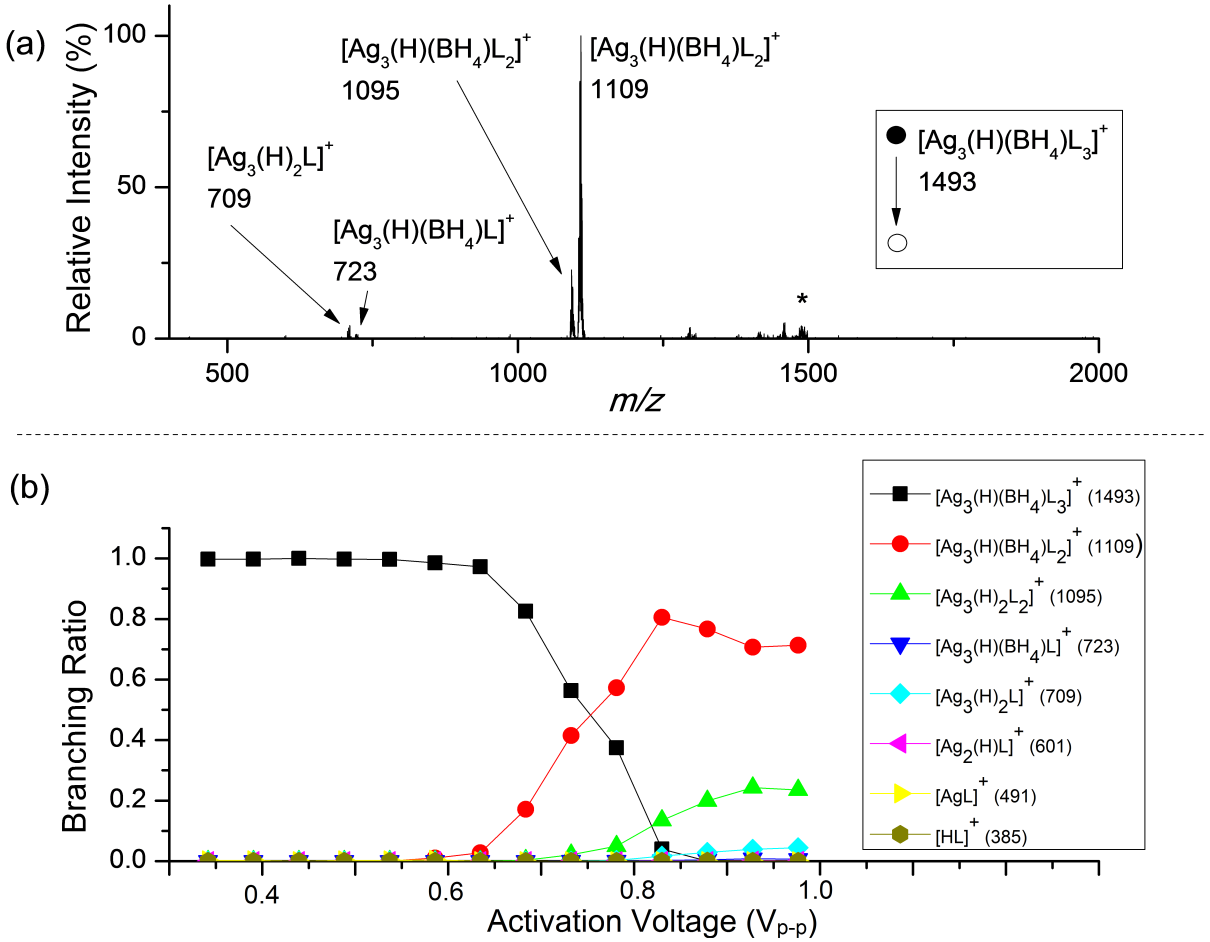

Figure S18: LCQ energy resolved CID of $[Ag_3(H)(BH_4)L_3]^+$. (a) CID spectrum at 0.92 volts. (b) branching ratio of products as a function of the activation amplitude used.

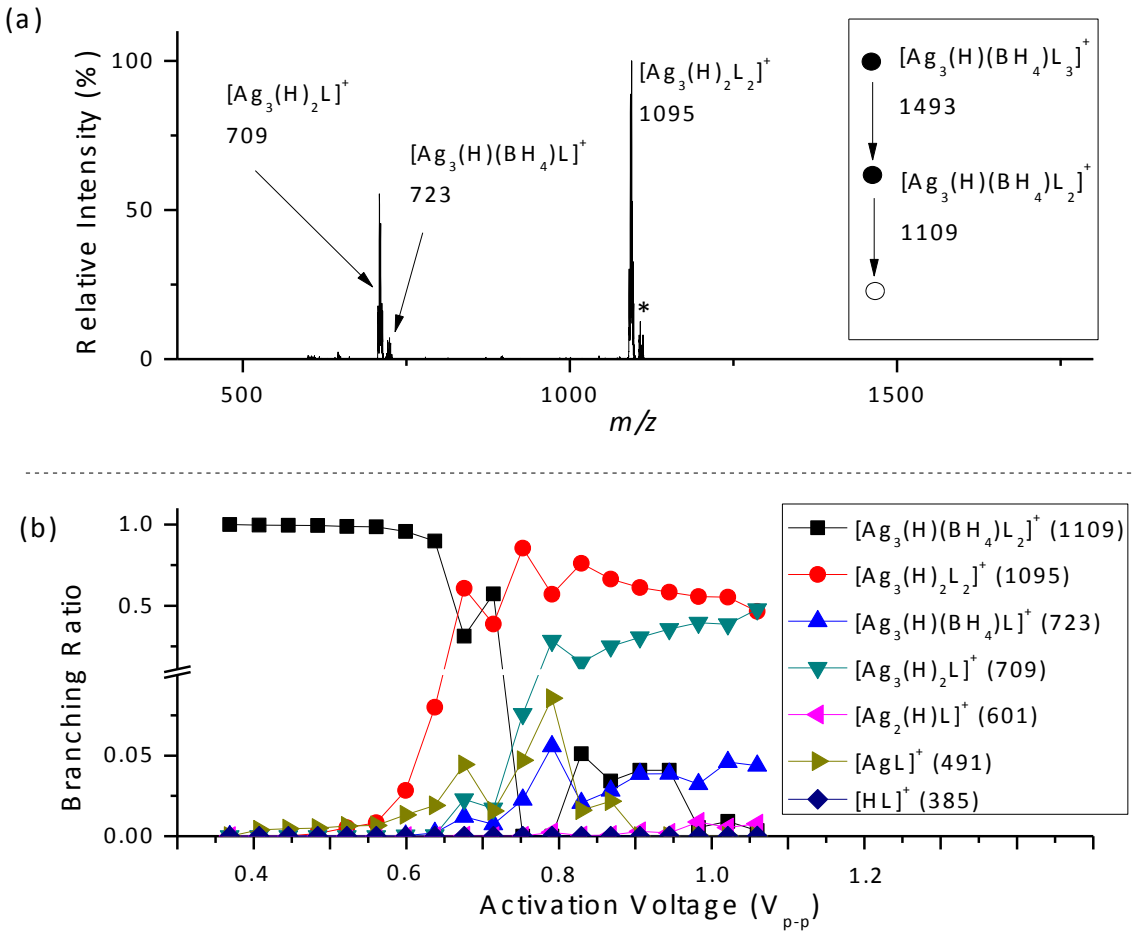

Figure S19: LCQ energy resolved CID of $[Ag_3(H)(BH_4)L_2]^+$. (a) CID spectrum at 0.90 volts. (b) branching ratio of products as a function of the activation amplitude used.

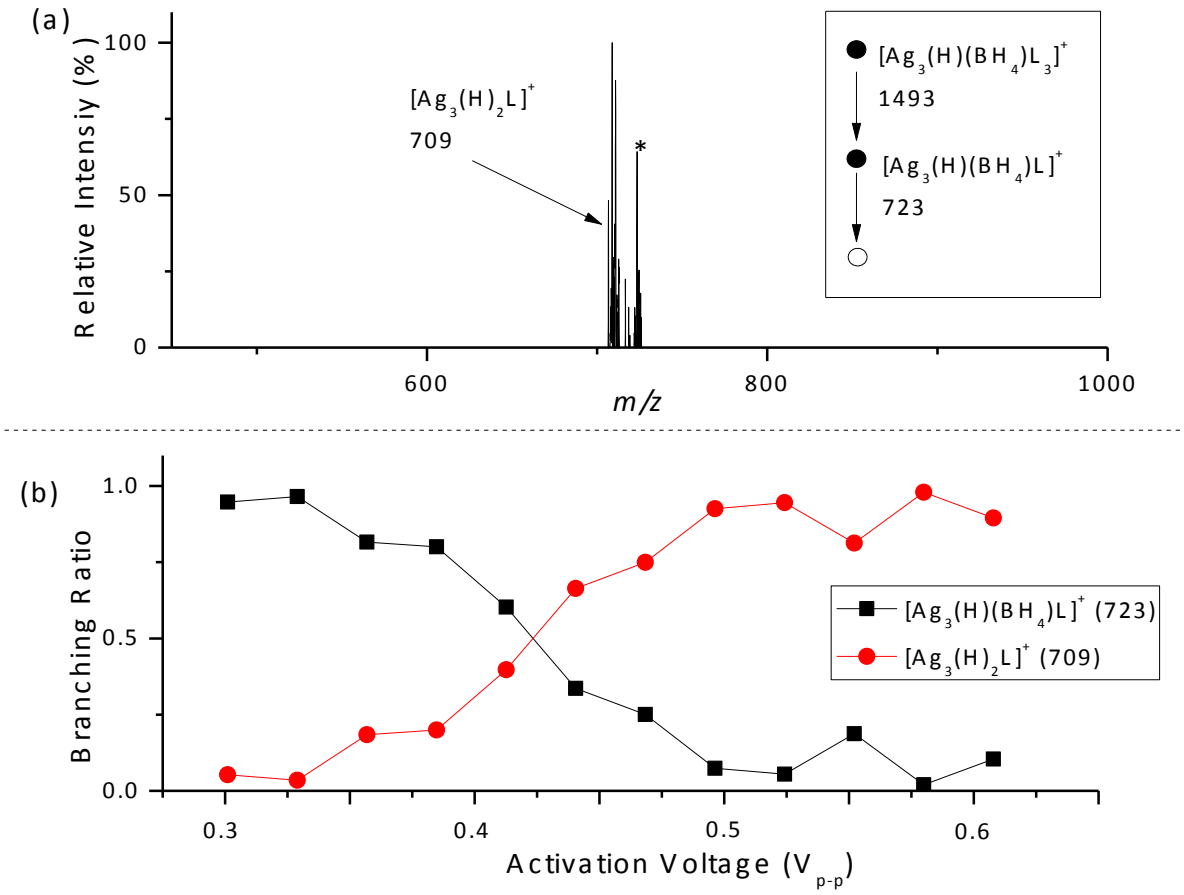

Figure S20: LCQ energy resolved CID of $[Ag_3(H)(BH_4)_2]^+$. (a) CID spectrum at 0.46 volts. (b) branching ratio of products as a function of the activation amplitude used.

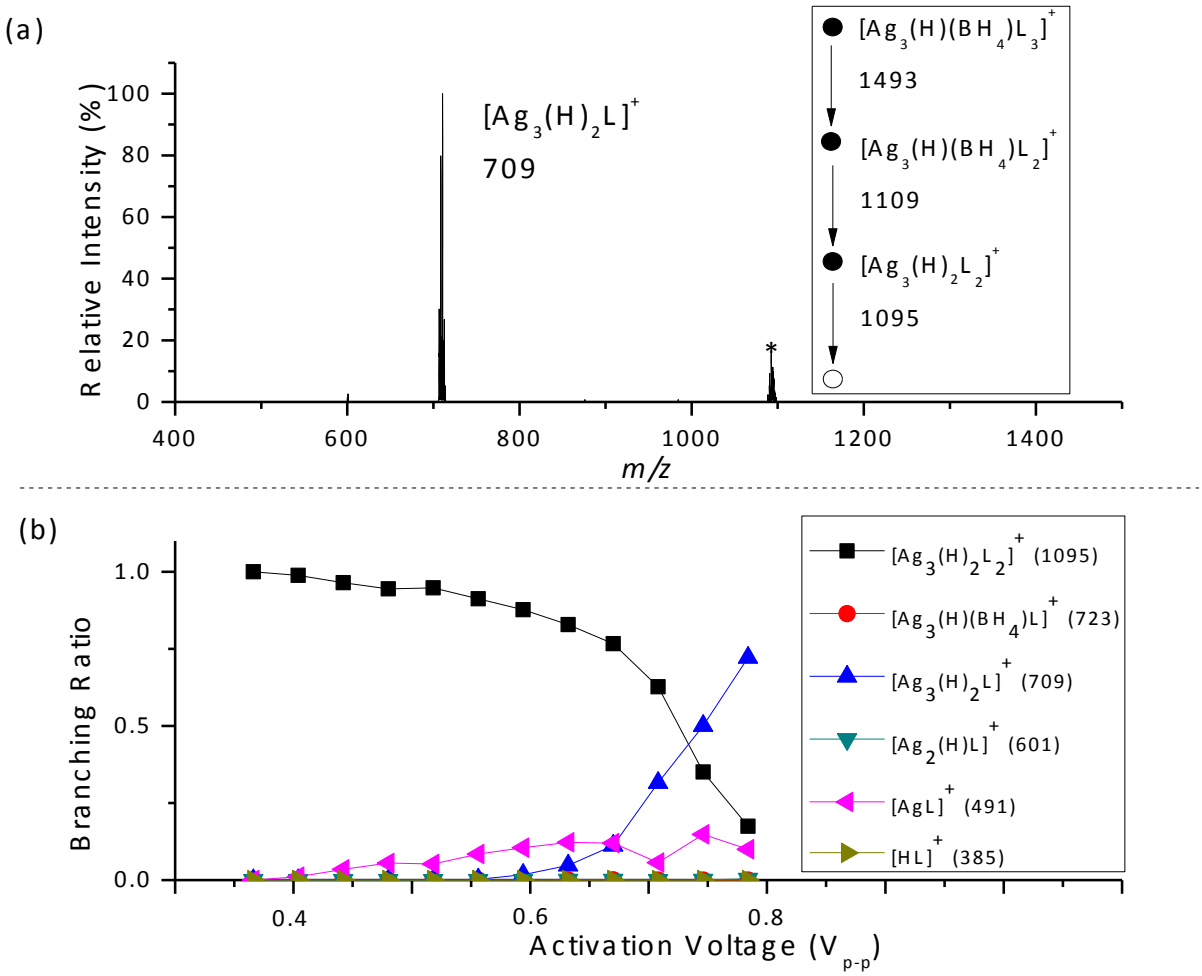

Figure S21: LCQ energy resolved CID of $[Ag_3(H)_2L_2]^+$. (a) CID spectrum at 0.76 volts. (b) branching ratio of products as a function of the activation amplitude used.

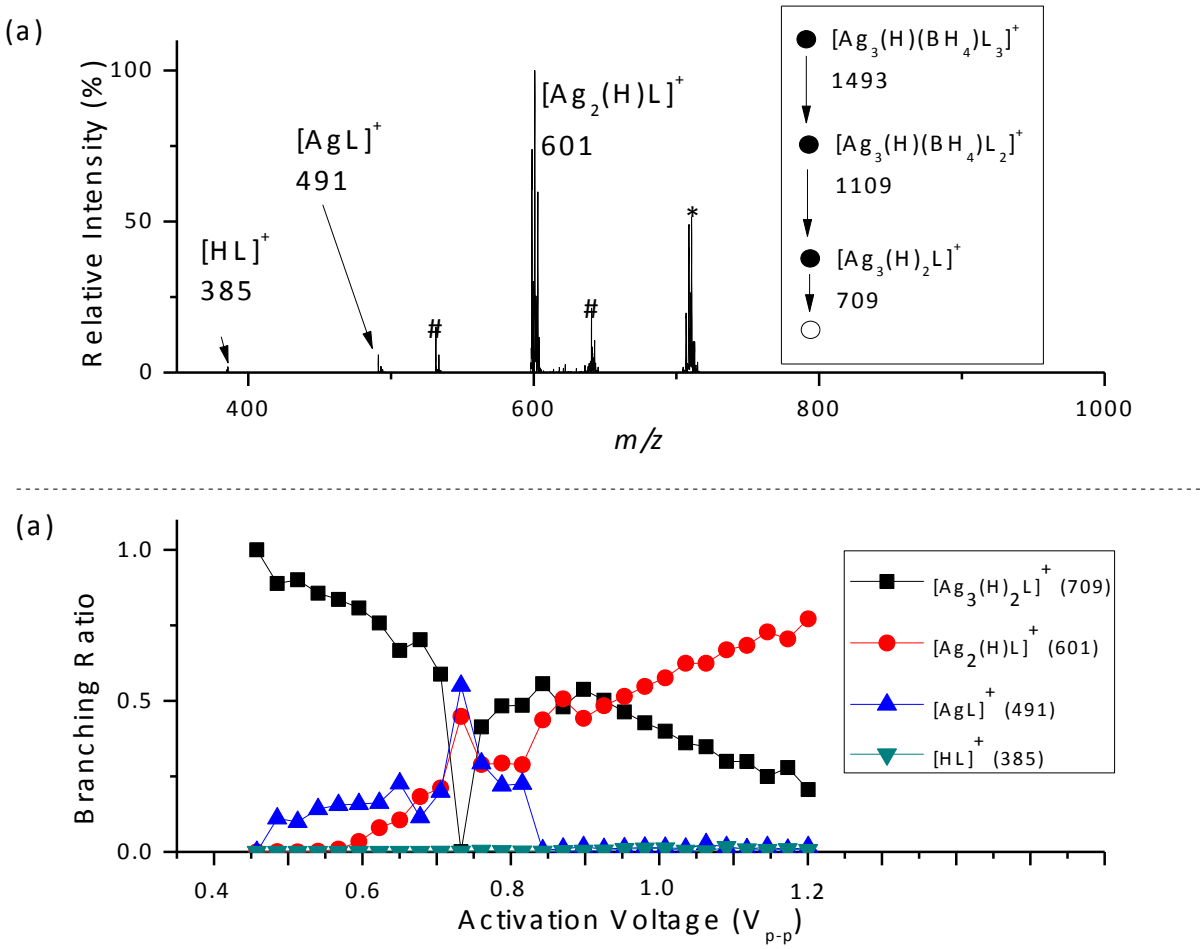

Figure S22: LCQ energy resolved CID of $[Ag_3(H)_2L]^+$. (a) CID spectrum at 1.04 volts. (b) branching ratio of products as a function of the activation amplitude used.

Cartesian coordinates and total energies for all of the calculated structures

$[Ag_3(H)(BH_4)L^{Me}{}_3]^+$

E(M06/BS1) = -3109.492746 au

H(M06/BS1) = -3108.855609 au

G(M06/BS1) = -3108.984256 au

E(M06/BS2//M06/BS1) = -3113.708582 au

C	-3.97746700	-0.36313700	0.79349200
H	-5.06071400	-0.56258900	0.83956100
H	-3.65612600	0.01562300	1.77535900
B	-0.01623900	-0.02847300	2.20560000
H	-1.05849000	0.53565300	1.81917100
H	0.00027600	-0.01769200	3.42388000
H	-0.02278700	-0.01383300	-1.35399800
Ag	-1.06204800	1.34923200	-0.32550700
P	-3.59226200	0.97080100	-0.42509200
P	-3.03609500	-1.93446300	0.49521000
H	0.00400400	-1.21247800	1.81790800
H	0.98892600	0.57697000	1.78816200
C	2.31496900	-3.22047900	0.86812600
H	3.04329300	-4.04521500	0.93438500
H	1.80713900	-3.12939600	1.83996700
Ag	-0.63989200	-1.61381200	-0.33211900
P	1.00342900	-3.58570100	-0.38205800
P	3.17978900	-1.60684900	0.56194100
C	1.71114200	3.59430200	0.81033600
H	2.06750800	4.63661500	0.84823700
H	1.94298800	3.11680500	1.77401900
Ag	1.69206200	0.23636500	-0.38177300
P	2.60058300	2.62987200	-0.48998900
P	-0.13575200	3.54306400	0.60947500
C	1.98159100	-3.85872700	-1.91465900
H	2.81740600	-4.55161000	-1.74270800
H	1.33280600	-4.27807800	-2.69269500
H	2.36650600	-2.90054600	-2.28658900
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H	-0.17692100	-5.70397000	-0.64526600
H	1.41865600	-5.96416300	0.10767900
H	0.06600200	-5.30353400	1.06832400
C	4.76832500	-2.13670800	-0.19856900
H	5.42621000	-1.26411700	-0.29412300
H	5.27363200	-2.89219400	0.41806900
H	4.60415400	-2.54465100	-1.20213600
C	3.71554400	-1.14848700	2.25575900
H	4.25166400	-1.97044600	2.74862100
H	4.37728700	-0.27460700	2.19854900
H	2.83382900	-0.87070800	2.84661100
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H	5.00712400	2.62199700	-0.88833700
H	4.50421400	4.15061700	-0.11855700
H	4.63532400	2.65553600	0.84879100
C	2.26978900	3.61187300	-2.00724000
H	2.49360100	4.67750500	-1.85716000
H	2.88866900	3.23495700	-2.82991000

H	1.21939000	3.49354400	-2.30264300
C	-0.49938100	5.20563100	-0.08999700
H	-1.58630100	5.34941400	-0.12807100
H	-0.06304600	6.00095000	0.52907300
H	-0.11262100	5.29475900	-1.11192700
C	-0.69503000	3.73635600	2.34602800
H	-0.21317200	4.59426500	2.83364800
H	-1.78286300	3.88093600	2.36213900
H	-0.46612600	2.81500000	2.89677200
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H	-5.81723300	1.89675000	0.10820000
H	-4.51885900	2.63903800	1.08516400
C	-4.35354400	0.34476700	-1.97557500
H	-5.36871300	-0.03970800	-1.80362700
H	-4.40720600	1.15988100	-2.70716200
H	-3.72784900	-0.44450900	-2.41073200
C	-4.27905900	-2.98521500	-0.36256600
H	-3.87516600	-3.99876800	-0.47347200
H	-5.21592900	-3.04089400	0.20802900
H	-4.49269200	-2.59729300	-1.36521800
C	-3.02245800	-2.67006500	2.17655200
H	-4.03207300	-2.72465100	2.60547200
H	-2.60250400	-3.68262600	2.12371500
H	-2.37707000	-2.06705000	2.82734800

$[Ag_3(H)(BH_4)L^{Me}{}_2]^+$

E(M06/BS1) = -2228.000079 au

H(M06/BS1) = -2227.556000 au

G(M06/BS1) = -2227.659437 au

E(M06/BS2//M06/BS1) = -2232.072635 au

C	3.52543500	0.63553100	1.06518700
H	4.53836300	1.04914200	1.19727900
H	3.11809100	0.39356000	2.05811900
B	-0.03440000	-0.92577500	2.19109600
H	1.10756600	-0.87279900	1.73871300
H	-0.00810200	-0.98808400	3.39992700
H	-0.23628300	-1.59905400	-1.64906500
Ag	1.37199300	-1.39535200	-0.85704800
P	3.59396400	-0.95238900	0.11909500
P	2.39794400	1.90376100	0.33540800
H	-0.72275900	0.10002400	1.92976600
H	-0.62276000	-1.94962400	1.77209700
C	-3.61950400	1.06935800	0.56658100
H	-4.60963700	1.50267600	0.35115200
H	-3.36523200	1.31508600	1.60862800
Ag	-0.00249100	1.14231700	0.26066400
P	-2.32248100	1.85356800	-0.49234800
P	-3.68005300	-0.78495500	0.43856000
Ag	-1.36867200	-1.56625100	-0.14988600
C	-2.85618400	1.46611200	-2.20256400
H	-3.91876500	1.70247300	-2.35195600
H	-2.26297000	2.06344400	-2.90503900
H	-2.67395500	0.40890500	-2.43288900

C	-2.75123400	3.63165200	-0.34193300
H	-2.10442300	4.22608800	-0.99782500
H	-3.79805600	3.81338900	-0.62015300
H	-2.59435600	3.96815700	0.68953500
C	-5.17831500	-1.07728400	-0.57814000
H	-5.37228200	-2.15452100	-0.63587700
H	-6.05460400	-0.58513300	-0.13585000
H	-5.03298000	-0.70737900	-1.59936600
C	-4.22829200	-1.26656400	2.11808900
H	-5.12783300	-0.71448000	2.42077500
H	-4.44808200	-2.34050300	2.13600500
H	-3.41988100	-1.07529800	2.83446300
C	4.10970800	-2.15233400	1.39918500
H	4.30936600	-3.12495400	0.93493000
H	5.01775100	-1.80939400	1.91205400
H	3.30147900	-2.27601800	2.12945500
C	5.09316900	-0.78680500	-0.92217400
H	5.96755400	-0.53129700	-0.30929900
H	5.28629000	-1.74056400	-1.42709300
H	4.95686300	-0.01946500	-1.69243900
C	3.22872200	2.35999900	-1.23586700
H	2.76246300	3.26730700	-1.63797900
H	4.29797900	2.55726500	-1.07723700
H	3.10646000	1.56788300	-1.98475500
C	2.75099000	3.35622300	1.39775400
H	3.82351800	3.59226100	1.39967700
H	2.19752500	4.22841500	1.03094800
H	2.42711900	3.15274000	2.42504900

$[Ag_3(H)_2L^{Me}_3]^+$

E(M06/BS1) = -3082.838167 au

H(M06/BS1) = -3082.236005 au

G(M06/BS1) = -3082.360653 au

E(M06/BS2//M06/BS1) = -3087.044329 au

C	0.32077800	3.60658200	-1.30541800
H	0.56269200	4.65452300	-1.54764300
H	0.05207600	3.08814100	-2.23749500
H	-0.68162100	0.38340600	-1.66917700
H	-0.40724600	0.21797300	1.60544500
Ag	-1.53893500	0.95984300	0.10344300
P	-1.16343500	3.48804500	-0.20362100
P	1.81182700	2.74457500	-0.61277400
C	3.56395700	-1.84375700	-0.37535800
H	4.36368000	-2.58337100	-0.19899100
H	3.84549900	-1.25156400	-1.26019700
Ag	1.23470600	0.65865500	0.87829600
P	3.44651100	-0.65314100	1.04106900
P	1.97309700	-2.68717000	-0.80493500
C	-3.70227300	-1.95544700	-0.26258500
H	-4.50668000	-2.57878800	0.16464500
H	-3.90067200	-1.84439800	-1.33993200
Ag	-0.10627500	-1.25341400	-1.08134800
P	-2.06705300	-2.81726200	-0.13106700
P	-3.76334900	-0.24273300	0.45133000

C	2.68673000	2.26834700	-2.16019900
H	3.69101900	1.89613500	-1.91954800
H	2.12792200	1.46313100	-2.65393000
H	2.78609100	3.11628200	-2.85145900
C	2.85147900	4.15410300	-0.03988500
H	2.39861600	4.64022900	0.83230700
H	3.83666600	3.77745200	0.26300800
H	2.98996500	4.90107300	-0.83326300
C	-2.30362800	4.65938600	-1.04798700
H	-2.58681800	4.26024600	-2.02899000
H	-3.21715600	4.77850800	-0.45356100
H	-1.84032500	5.64626900	-1.18326600
C	-0.63298700	4.49104300	1.24513500
H	0.13055200	3.94651200	1.81518500
H	-0.23827800	5.46958300	0.93646300
H	-1.48738300	4.65208300	1.91295900
C	-5.36774000	0.32896100	-0.24640200
H	-5.64062200	1.29134100	0.20289600
H	-5.27536200	0.47274900	-1.32911500
H	-6.17110300	-0.39323700	-0.04645400
C	-4.25044400	-0.54609600	2.19941200
H	-3.39418500	-0.89658500	2.78593900
H	-4.58391300	0.40234800	2.63803200
H	-5.06996500	-1.27444200	2.27482400
C	-1.93854700	-3.15510700	1.67561200
H	-1.61826100	-2.24871400	2.20537200
H	-2.88971900	-3.51524900	2.09302900
H	-1.17695800	-3.92806700	1.84139400
C	-2.54504100	-4.48676900	-0.75312900
H	-2.81975600	-4.42967800	-1.81297400
H	-1.69593400	-5.17577400	-0.66093700
H	-3.39280200	-4.89912500	-0.18907100
C	1.72937400	-3.83788800	0.60854000
H	0.97886300	-4.58647300	0.32102400
H	2.65487800	-4.35999500	0.88914200
H	1.33599000	-3.28716900	1.47347800
C	2.53571600	-3.83950400	-2.12082300
H	3.37561600	-4.45913800	-1.77925400
H	1.70579600	-4.49507700	-2.41137600
H	2.84457300	-3.27421200	-3.00763700
C	5.05220900	0.23000000	0.86894200
H	5.18706500	0.91038400	1.71846400
H	5.89751400	-0.47095500	0.84175200
H	5.05912200	0.82869100	-0.05001400
C	3.80890700	-1.70244300	2.50761600
H	4.68520300	-2.34282900	2.33597400
H	4.01588700	-1.04835700	3.36322400
H	2.94828300	-2.32603100	2.77053600

$[Ag_3(H)_2L^{Me}{}_2]^+$
E(M06/BS1) = -2201.358866 au
H(M06/BS1) = -2200.950546 au
G(M06/BS1) = -2201.049756 au
E(M06/BS2//M06/BS1) = -2205.421185 au

C	-3.69818300	0.61344000	-0.67045800
H	-4.69083200	1.04474900	-0.45772900
H	-3.67123500	0.34775000	-1.73823700
H	0.50430200	-2.33522700	0.87657300
Ag	-1.14213600	-1.69924800	0.49701000
P	-3.48877300	-0.96307400	0.27340800
P	-2.36871900	1.87889600	-0.42529300
H	0.44894700	-0.48196200	-1.94541600
C	3.57250000	1.27458000	0.07352800
H	4.36611600	1.69516400	0.71379200
H	3.71242000	1.68179500	-0.93941300
Ag	-0.05519700	0.96620900	-0.86814000
P	1.90474800	1.85529900	0.64126600
P	3.76549500	-0.57118900	-0.06253200
Ag	1.43715800	-1.43947800	-0.57573300
C	1.80558800	1.21758900	2.36365000
H	2.70702700	1.46485500	2.94222400
H	0.93773100	1.67140900	2.85969600
H	1.65382300	0.13062800	2.36179900
C	2.24496300	3.63869400	0.93792000
H	1.35902700	4.11364500	1.37699300
H	3.09254400	3.77410600	1.62330200
H	2.46874200	4.14455600	-0.00833500
C	4.56591100	-1.01039600	1.53133100
H	4.87201100	-2.06265600	1.49972200
H	5.45300500	-0.39004800	1.71801200
H	3.86074000	-0.89515900	2.36176000
C	5.17975500	-0.68769300	-1.22701900
H	6.01896600	-0.06317600	-0.89290800
H	5.51815300	-1.72847100	-1.28964000
H	4.86842800	-0.37064800	-2.22872000
C	-4.59534800	-2.09970400	-0.64187200
H	-4.67105300	-3.05241000	-0.10502700
H	-5.59979400	-1.66810900	-0.74385900
H	-4.18603500	-2.30155500	-1.63810800
C	-4.42248400	-0.67560000	1.82480000
H	-5.44016400	-0.32390800	1.60860900
H	-4.48781500	-1.61850400	2.38040800
H	-3.91627800	0.05558900	2.46443400
C	-2.60358200	2.41457900	1.31673600
H	-2.03609300	3.34063300	1.47617900
H	-3.65909700	2.60891600	1.55330100
H	-2.20178200	1.66125700	2.00696200
C	-3.06998100	3.29626000	-1.35545600
H	-4.07444900	3.55089600	-0.99209300
H	-2.41980900	4.17119200	-1.24070100
H	-3.12544200	3.05351900	-2.42273100

$[Ag_3(H)(BH_4)L^{Me}]^+$
E(M06/BS1) = -1346.503099 au
H(M06/BS1) = -1346.252796 au
G(M06/BS1) = -1346.328975 au
E(M06/BS2//M06/BS1) = -1350.434988 au

C	2.77304200	0.44787800	-0.70082800
H	3.84707500	0.61820200	-0.51927800
H	2.59451000	0.58715900	-1.77755000
B	-3.00308700	1.72117500	-0.55017900
H	-2.49878700	2.03314500	0.55214400
H	-3.68305700	2.65193700	-0.88278900
H	-1.76354300	-2.07393000	0.60169200
Ag	-0.62439200	1.58915600	-0.21635500
P	1.77580900	1.73168200	0.17333300
P	2.33871100	-1.30282300	-0.29713400
H	-2.22756900	1.49915500	-1.51097700
H	-3.84580500	0.78856700	-0.42172500
Ag	-0.05758400	-1.62705800	0.17695000
Ag	-2.71306200	-0.63870500	0.11998900
C	2.57892800	3.28527100	-0.35670800
H	2.10385300	4.13446000	0.14803200
H	3.64810500	3.27687400	-0.10771500
H	2.46061400	3.42276100	-1.43748000
C	2.25740400	1.57696700	1.93091900
H	3.34975700	1.53883400	2.04024200
H	1.88257500	2.45016900	2.47826000
H	1.80673900	0.68712100	2.38712900
C	3.47537900	-1.75476600	1.06441200
H	3.37805400	-2.82707300	1.27081400
H	4.51608800	-1.54519300	0.78429300
H	3.23211000	-1.21237200	1.98442100
C	3.01622600	-2.22316400	-1.72417000
H	4.07510000	-1.97656000	-1.87547300
H	2.92754200	-3.30023300	-1.54094700
H	2.45515700	-1.98435300	-2.63438800

$[Ag_3(H)_2\ L^{Me}]^+$

E(M06/BS1) = -1319.874473 au

H(M06/BS1) = -1319.659579 au

G(M06/BS1) = -1319.730716 au

E(M06/BS2//M06/BS1) = -1323.792176 au

C	2.57420300	0.00000700	-0.73664800
H	3.67526200	0.00001300	-0.66019700
H	2.32387200	0.00000100	-1.80881400
H	-2.36307400	-1.81378300	0.01483500
Ag	-0.53275500	1.75070900	-0.01074100
P	1.92552200	1.59422200	-0.05709700
P	1.92553700	-1.59421200	-0.05708800
H	-2.36309000	1.81376400	0.01491800
Ag	-0.53273900	-1.75070600	-0.01073800
Ag	-2.69224700	-0.00001100	0.01999200
C	2.79443600	2.80749200	-1.11634200
H	2.57080200	3.82279000	-0.76902100
H	3.88047900	2.65173500	-1.07689100
H	2.45488800	2.72097600	-2.15454300
C	2.76480000	1.79666000	1.55632200
H	3.83696200	1.57353000	1.47327800
H	2.64987000	2.83740000	1.88245900
H	2.31630400	1.16017600	2.32584800

C	2.76484300	-1.79665700	1.55631400
H	2.64993400	-2.83740500	1.88243700
H	3.83700200	-1.57351100	1.47325500
H	2.31635300	-1.16019200	2.32585700
C	2.79442800	-2.80747700	-1.11635500
H	3.88047100	-2.65171300	-1.07694100
H	2.57081200	-3.82277600	-0.76902300
H	2.45484500	-2.72096900	-2.15454600

$[Ag_3(H)(BH_4)]^+$

E(M06/BS1) = -464.9514358 au

H(M06/BS1) = -464.896099 au

G(M06/BS1) = -464.945194 au

E(M06/BS2//M06/BS1) = -468.728454 au

B	-1.61211900	0.10699200	-0.00489400
H	-2.16990200	-0.32646200	-1.03259000
H	-1.19496000	1.22137900	-0.32689900
H	2.43333200	1.11782800	-0.06039000
Ag	-3.95820800	-0.19732000	-0.00008400
H	-2.24649000	0.29880400	1.05155600
H	-0.82921000	-0.80479600	0.29407400
Ag	3.46187400	-0.33977700	-0.00008400
Ag	0.75309700	0.49365700	0.00226800

L^{Me}

E(M06/BS1) = -881.4273069 au

H(M06/BS1) = -881.235789 au

G(M06/BS1) = -881.285286 au

E(M06/BS2//M06/BS1) = -881.5738711 au

C	0.00312500	-0.73330400	0.21312300
H	0.02496600	-0.55105100	1.30301000
H	-0.08841400	-1.82033900	0.06500200
P	1.60005000	-0.22672900	-0.60293900
P	-1.51487300	0.04014800	-0.55846900
C	2.76542600	-0.91358000	0.67191400
H	3.79286800	-0.60506400	0.44095300
H	2.51732700	-0.57276300	1.68770600
H	2.73496900	-2.01000900	0.65393000
C	1.67505000	1.54994600	-0.06831800
H	1.42201600	1.67762900	0.99508700
H	2.69123100	1.93075000	-0.23174800
H	0.99595300	2.16149400	-0.67515400
C	-1.78265900	1.44741400	0.62506000
H	-2.77811600	1.87600600	0.45220500
H	-1.72101100	1.12070800	1.67369900
H	-1.04700500	2.24374800	0.46185500
C	-2.77624600	-1.11506200	0.16918500
H	-2.63021100	-1.25381900	1.25037100
H	-3.78492300	-0.71741500	0.00085400
H	-2.71546500	-2.09365600	-0.32244800

BH_3

E(M06/BS1) = -26.582141 au

H(M06/BS1) = -26.551922 au

G(M06/BS1) = -26.574995 au

E(M06/BS2//M06/BS1) = -26.594077 au

E(B3LYP-D3BJ/BS2//M06/BS1) = -26.625207 au

B	0.00015600	0.00001000	-0.00003800
H	-0.60766600	-1.02353700	0.00006300
H	-0.58345700	1.03747200	0.00006300
H	1.19034500	-0.01398600	0.00006300

$[Ag_3(H)(BH_4)L^{Ph}_3]^+$

E(M06/BS1) = -5408.503573 au

H(M06/BS1) = -5407.186337 au

G(M06/BS1) = -5407.398341 au

E(M06/BS2//M06/BS1) = -5413.533698 au

E(B3LYP-D3BJ/BS2//M06/BS1) = -5416.591986 au

C	3.68616500	-1.26909300	0.99319100
H	4.73727500	-1.58118000	1.08180400
H	3.22382100	-1.31528500	1.99024600
B	-0.01174500	0.05997400	2.42879100
H	0.60064700	-0.92112200	1.96641200
H	0.10944700	0.02953700	3.64241500
H	-0.18314400	0.04741100	-1.12840100
Ag	0.26851600	-1.61287500	-0.15355400
P	2.68759200	-2.38501800	-0.09298800
P	3.55578000	0.50306400	0.43824400
H	0.47855000	1.12213100	2.01083200
H	-1.22982300	-0.01338300	2.16571600
C	-0.70620700	3.91417200	1.13768300
H	-0.91230300	4.98564200	1.28210700
H	-0.37137500	3.48589300	2.09484500
Ag	1.16606800	1.14814000	-0.19344100
P	0.68874000	3.63340000	-0.04370100
P	-2.22933300	2.95611900	0.69661900
C	-3.01246900	-2.73664000	1.06209500
H	-3.77919200	-3.52442500	1.09966900
H	-2.88059000	-2.33314100	2.07670300
Ag	-1.74578700	0.53699100	0.08171100
P	-3.50855800	-1.31498500	-0.01542400
P	-1.36390200	-3.42623400	0.53515200
C	4.10294900	1.42079000	1.92423300
C	5.13202000	2.36496900	1.87870200
C	3.38614500	1.24264900	3.11530300
C	5.46195100	3.09489500	3.01673900
H	5.67917300	2.53485800	0.95209300
C	3.72583700	1.97012600	4.24934400
H	2.53907900	0.55464500	3.15850200
C	4.76894800	2.89193400	4.20506100
H	6.26675200	3.82711400	2.96959800
H	3.16845000	1.81552300	5.17163600
H	5.03493600	3.45936100	5.09567100
C	4.91370300	0.68392400	-0.76707200

C	6.23494800	0.33434100	-0.46269200
C	4.61259400	1.17679400	-2.03830900
C	7.23501200	0.47805800	-1.41509900
H	6.48593400	-0.03478500	0.53307700
C	5.61482700	1.31688100	-2.99453500
H	3.58077500	1.44459900	-2.27819300
C	6.92370500	0.96677600	-2.68296200
H	8.26140700	0.21057300	-1.16996400
H	5.37075200	1.69652300	-3.98509800
H	7.70823900	1.07827700	-3.42946700
C	2.02529800	4.68113300	0.63308400
C	3.00677100	5.15915200	-0.24306200
C	2.15791500	4.92253400	2.00299300
C	4.08622300	5.88848400	0.24140300
H	2.91551800	4.97092400	-1.31435100
C	3.24087900	5.65234500	2.48351100
H	1.42233500	4.54001700	2.71032900
C	4.20143900	6.14238400	1.60542100
H	4.83529700	6.26800700	-0.45151300
H	3.33285500	5.83526200	3.55287900
H	5.04404600	6.71862800	1.98391100
C	0.19155600	4.47891200	-1.58253800
C	-0.20035900	5.82191600	-1.60310300
C	0.20808800	3.74891700	-2.77314200
C	-0.57740900	6.42007300	-2.79796700
H	-0.20016700	6.40627600	-0.68154600
C	-0.16204000	4.35224500	-3.97271100
H	0.50662400	2.69815600	-2.75247200
C	-0.55594900	5.68546700	-3.98280400
H	-0.88227800	7.46495200	-2.80979700
H	-0.14405400	3.77920000	-4.89813400
H	-0.84653600	6.15967900	-4.91873500
C	-3.09858000	3.99456300	-0.53062800
C	-3.58812500	5.26678400	-0.21721200
C	-3.28137300	3.48410900	-1.81734200
C	-4.24207600	6.01929500	-1.18447000
H	-3.47015000	5.66357600	0.79275800
C	-3.93960700	4.23776900	-2.78507100
H	-2.90276300	2.48657200	-2.05650700
C	-4.41648600	5.50496600	-2.46810500
H	-4.62547500	7.00754700	-0.93649800
H	-4.07747100	3.83420600	-3.78678500
H	-4.93405400	6.09482300	-3.22268200
C	-3.26048400	3.10490400	2.19757000
C	-4.43262900	2.34027700	2.23163400
C	-2.94391900	3.91561500	3.28906000
C	-5.27616000	2.39666000	3.33337400
H	-4.69208900	1.69636600	1.38727500
C	-3.78504000	3.96088400	4.39773500
H	-2.03760200	4.52013300	3.28607100
C	-4.95037100	3.20350500	4.42099400
H	-6.18535800	1.79773500	3.34223300
H	-3.52568000	4.59190500	5.24594100
H	-5.60519100	3.23854900	5.28972900
C	-5.21514800	-0.92215300	0.50530500
C	-5.93289000	-0.02737900	-0.29999800

C	-5.78213700	-1.36735000	1.70045200
C	-7.19897800	0.39976600	0.07666000
H	-5.49006600	0.34122000	-1.22855600
C	-7.05182400	-0.93415200	2.07829300
H	-5.24099700	-2.05498900	2.34890700
C	-7.76137100	-0.05375000	1.26935600
H	-7.74955200	1.09057400	-0.55909800
H	-7.48646300	-1.29246400	3.00997400
H	-8.75356200	0.28117700	1.56601400
C	-3.72825800	-2.06346900	-1.66957200
C	-4.58016600	-3.15373200	-1.87967800
C	-3.00471800	-1.53931200	-2.74350200
C	-4.68569800	-3.72478000	-3.14074900
H	-5.16037300	-3.56280000	-1.05070300
C	-3.12232200	-2.10430100	-4.01147800
H	-2.33551100	-0.69210500	-2.57678400
C	-3.95594600	-3.19976600	-4.20676900
H	-5.33945000	-4.58128400	-3.29560900
H	-2.56018300	-1.68799400	-4.84571300
H	-4.04597100	-3.64606500	-5.19589900
C	-0.76322500	-4.27052000	2.04131100
C	-0.34249400	-5.60283100	2.03515800
C	-0.59617200	-3.50266400	3.20174700
C	0.19757900	-6.16969100	3.18592200
H	-0.43202800	-6.20325600	1.13025700
C	-0.05994500	-4.07609700	4.34754400
H	-0.86003000	-2.44351500	3.21016700
C	0.33105900	-5.41297100	4.34436800
H	0.51382700	-7.21170900	3.17305300
H	0.05641500	-3.47126400	5.24499600
H	0.74821300	-5.86129100	5.24454100
C	-1.80201900	-4.74379100	-0.64796600
C	-2.65540100	-5.80229300	-0.31308500
C	-1.28704500	-4.66511400	-1.94377400
C	-2.97893200	-6.76738900	-1.25848200
H	-3.05671900	-5.88161800	0.69863000
C	-1.61766300	-5.62812200	-2.89282600
H	-0.64090200	-3.82661200	-2.21551700
C	-2.45866700	-6.68080000	-2.54886500
H	-3.63570400	-7.59260900	-0.98896100
H	-1.21881700	-5.55223200	-3.90304300
H	-2.71307700	-7.43801300	-3.28848700
C	3.55992900	-2.37400700	-1.69839200
C	4.90541000	-2.73875800	-1.81168000
C	2.85448200	-1.98592500	-2.84005700
C	5.53802800	-2.69951600	-3.04692800
H	5.45974600	-3.06181100	-0.92887800
C	3.48721700	-1.95733600	-4.08087600
H	1.80485000	-1.69530900	-2.74859800
C	4.82811900	-2.31079300	-4.18202200
H	6.58776400	-2.97608700	-3.12790000
H	2.93068400	-1.65919800	-4.96782800
H	5.32519700	-2.28766200	-5.15035300
C	2.98613100	-4.06566100	0.55590100
C	2.53253500	-5.13564800	-0.22660900
C	3.54936000	-4.32680100	1.80618900

C	2.66784900	-6.44239500	0.22156300
H	2.07964600	-4.94369700	-1.20213500
C	3.67111100	-5.63869700	2.25861400
H	3.90124600	-3.51211300	2.43795600
C	3.24168900	-6.69631500	1.46588100
H	2.32660800	-7.26676500	-0.40258000
H	4.11527800	-5.83079800	3.23388600
H	3.34852400	-7.72067000	1.81896900

$[Ag_3(H)(BH_4)L^{Ph}_2]^+$

E(M06/BS1) = -3760.671618 au

H(M06/BS1) = -3759.774952 au

G(M06/BS1) = -3759.936572 au

E(M06/BS2//M06/BS1) = -3765.285290 au

E(B3LYP-D3BJ/BS2//M06/BS1) = -3767.347609 au

C	3.50633200	-0.16415800	1.16098600
H	4.50558400	0.20280000	1.43647600
H	3.06990300	-0.67696200	2.03106200
B	-0.09044200	-1.80449600	2.00925600
H	0.97953200	-1.71979500	1.39348600
H	0.15860500	-2.12968900	3.15045600
H	-0.30582100	-1.99452100	-1.90040300
Ag	1.30411100	-1.77829600	-1.11211100
P	3.58069400	-1.41426400	-0.20091700
P	2.35811700	1.23837100	0.78046400
H	-0.71625900	-0.71517100	2.09309000
H	-0.83078300	-2.66748900	1.49731100
C	-3.57384200	0.57284400	0.92671600
H	-4.52699500	1.12166300	0.92678800
H	-3.23108300	0.47754500	1.96834400
Ag	-0.00302300	0.46594100	0.49790900
P	-2.24349400	1.51704400	0.04495300
P	-3.75168400	-1.15269500	0.25755500
Ag	-1.47459800	-1.98158200	-0.42908900
C	-2.23596700	3.13154100	0.90147700
C	-2.79627800	4.29777000	0.37754200
C	-1.56663000	3.18177100	2.13237400
C	-2.69705400	5.49474600	1.08157400
H	-3.30047100	4.27898300	-0.58794500
C	-1.47699200	4.37613600	2.83529200
H	-1.09969500	2.28031800	2.54170600
C	-2.04232300	5.53510200	2.30784900
H	-3.13150300	6.40195600	0.66571400
H	-0.95523200	4.40435400	3.79010300
H	-1.96540500	6.47434300	2.85226100
C	-4.54108400	-2.06863100	1.61817400
C	-4.28027300	-3.43981700	1.69806100
C	-5.39164800	-1.47635300	2.55800100
C	-4.87344200	-4.21147100	2.69025300
H	-3.59660600	-3.90226200	0.98422100
C	-5.97759400	-2.24906000	3.55409400
H	-5.59787600	-0.40615500	2.52364300
C	-5.72182200	-3.61592900	3.61827700
H	-4.66213500	-5.27732400	2.74613500

H	-6.63598700	-1.78218200	4.28415800
H	-6.18056000	-4.21746600	4.40050400
C	-2.89016700	1.78169900	-1.63356300
C	-4.20645700	2.19587000	-1.87450700
C	-2.04325900	1.52388200	-2.71503000
C	-4.66088600	2.35554200	-3.17688500
H	-4.88709900	2.38248000	-1.04272300
C	-2.49953500	1.68775200	-4.01969800
H	-1.02743200	1.16952700	-2.53092200
C	-3.80648300	2.10442300	-4.24892000
H	-5.68826100	2.66602600	-3.35759900
H	-1.83558700	1.48102600	-4.85675000
H	-4.16741600	2.22752700	-5.26842900
C	-5.00819900	-1.00239300	-1.05913100
C	-6.33469700	-0.64979100	-0.78765300
C	-4.61316400	-1.23137600	-2.37907800
C	-7.24600400	-0.51252300	-1.82701700
H	-6.66364900	-0.49913100	0.24162600
C	-5.52816300	-1.09532900	-3.41845600
H	-3.57677500	-1.50100400	-2.59303400
C	-6.84289300	-0.73548000	-3.14264000
H	-8.27844700	-0.24413400	-1.61040000
H	-5.21175900	-1.27235400	-4.44487700
H	-7.56221400	-0.63447400	-3.95340700
C	4.24925600	-2.91123500	0.59065400
C	4.03118200	-4.12884200	-0.06270800
C	4.97711600	-2.89325000	1.78398000
C	4.54255400	-5.30902300	0.46283500
H	3.45283000	-4.15281600	-0.98860800
C	5.48051500	-4.07763700	2.31140800
H	5.15538100	-1.95820200	2.31475800
C	5.26597300	-5.28347800	1.65175400
H	4.36702400	-6.25203900	-0.05083300
H	6.04253100	-4.05744500	3.24303200
H	5.65934400	-6.20867500	2.06818600
C	4.89314500	-0.81537500	-1.31439800
C	6.22791200	-0.76554400	-0.89691300
C	4.55261500	-0.38235600	-2.59685100
C	7.20478300	-0.26859200	-1.74977300
H	6.50591200	-1.13311500	0.09216400
C	5.53247900	0.11948600	-3.44770000
H	3.51346900	-0.43386000	-2.92690700
C	6.85618700	0.17618300	-3.02381000
H	8.24350500	-0.23826600	-1.42626100
H	5.26152300	0.45958200	-4.44546500
H	7.62409300	0.55992500	-3.69311500
C	2.42836800	2.23641000	2.30834200
C	2.94984700	3.53045600	2.35306900
C	1.84986700	1.68247600	3.45927500
C	2.90790500	4.25728800	3.54007200
H	3.38707500	3.97670300	1.46041600
C	1.82243200	2.40830500	4.64349700
H	1.41507900	0.67982000	3.43228600
C	2.35158300	3.69728700	4.68480400
H	3.31750200	5.26524300	3.56876600
H	1.38362900	1.96745200	5.53683200

H	2.32765200	4.26588400	5.61259900
C	3.18420200	2.19033800	-0.53043000
C	4.55472400	2.47594100	-0.50118800
C	2.41660700	2.62015000	-1.61631200
C	5.14596800	3.16978300	-1.54850300
H	5.16665800	2.15384100	0.34253900
C	3.00861700	3.32483700	-2.66050600
H	1.34827800	2.39669500	-1.63784800
C	4.37233600	3.59514600	-2.62751100
H	6.21361300	3.37956600	-1.52476800
H	2.40416900	3.65944500	-3.50134100
H	4.83894400	4.13942500	-3.44656700

$[Ag_3(H)_2L^{Ph}{}_3]^+$

E(M06/BS1) = -5381.859998 au

H(M06/BS1) = -5380.577766 au

G(M06/BS1) = -5380.779571 au

E(M06/BS2//M06/BS1) = -5386.877760 au

E(B3LYP-D3BJ/BS2//M06/BS1) = -5389.905173 au

C	3.22338900	1.25157600	1.49458000
H	4.09480700	1.76418500	1.92775500
H	2.61113300	0.83753500	2.30755900
H	0.72527500	-0.71182700	1.53989600
H	0.58782500	-0.34978800	-1.86190900
Ag	1.46324900	-1.24625100	-0.33328900
P	3.68397700	-0.18478000	0.41375800
P	2.17043000	2.46226900	0.54625900
C	-2.51825100	2.96031300	0.49444200
H	-3.44946900	3.53894500	0.39497100
H	-1.89791700	3.41391700	1.28424100
Ag	0.44364400	1.32152800	-1.08188100
P	-1.50559300	3.00516500	-1.05531800
P	-2.88105300	1.22905900	1.04202500
C	-0.64743500	-4.02630400	0.71630100
H	-1.01424900	-5.05930600	0.62173300
H	-0.36366900	-3.86018300	1.76538400
Ag	-0.97213000	-0.39410700	0.96449000
P	-1.95744000	-2.77349600	0.31518000
P	0.92722800	-3.73595800	-0.24102700
C	1.19310500	3.30836700	1.84852000
C	0.96641800	4.68823400	1.79919700
C	0.49182800	2.54047800	2.79002300
C	0.07462500	5.28705100	2.68694100
H	1.48145700	5.30516600	1.06147100
C	-0.39775200	3.14175200	3.67376300
H	0.61168400	1.45555600	2.81635100
C	-0.60815000	4.51922200	3.62490700
H	-0.08407900	6.36352400	2.63890400
H	-0.93627500	2.52960400	4.39769000
H	-1.30574900	4.98877000	4.31744700
C	3.38287500	3.70029800	-0.03032700
C	4.19853200	4.42739700	0.84481900
C	3.51429000	3.89403100	-1.40669700
C	5.13018200	5.32927300	0.34587300

H	4.09367900	4.29547300	1.92299400
C	4.44967900	4.79590300	-1.90641100
H	2.89337700	3.31479900	-2.09291500
C	5.25597200	5.51340200	-1.03008300
H	5.75930400	5.89407900	1.03160700
H	4.55281100	4.93048300	-2.98188800
H	5.98809900	6.21936200	-1.41820900
C	-1.01434000	4.76167800	-1.18964000
C	0.04746300	5.04615800	-2.05533100
C	-1.59192300	5.80217400	-0.45817700
C	0.51871000	6.34618700	-2.19389300
H	0.51569200	4.23620800	-2.62037500
C	-1.11173500	7.10176400	-0.58793500
H	-2.41285700	5.60533000	0.23122000
C	-0.05761800	7.37530600	-1.45406200
H	1.34591600	6.55565700	-2.86969200
H	-1.56635600	7.90488600	-0.01015500
H	0.31670000	8.39259900	-1.55150600
C	-2.72400200	2.73863000	-2.39384200
C	-3.93192800	3.44034700	-2.45986300
C	-2.43221000	1.78230800	-3.36949400
C	-4.83978100	3.17516200	-3.47660400
H	-4.16613200	4.20407500	-1.71643800
C	-3.33896300	1.52338000	-4.39339500
H	-1.49400300	1.22450300	-3.31165000
C	-4.54338500	2.21639000	-4.44411300
H	-5.78006400	3.72161500	-3.52092700
H	-3.10368200	0.77614700	-5.14967800
H	-5.25544200	2.01402900	-5.24226000
C	-4.32399400	0.73279900	0.03700300
C	-5.63665500	1.07157700	0.37437700
C	-4.08312200	-0.03445700	-1.10579100
C	-6.69131500	0.64213700	-0.42485600
H	-5.83596300	1.65703300	1.27318200
C	-5.13607000	-0.45307700	-1.91201100
H	-3.06014300	-0.32187100	-1.35758400
C	-6.44276000	-0.11899300	-1.56576300
H	-7.71394900	0.90002100	-0.15477000
H	-4.92825900	-1.05586500	-2.79637800
H	-7.27370400	-0.45507200	-2.18357400
C	-3.52545700	1.42301800	2.73620300
C	-3.61835600	0.25780100	3.50702000
C	-3.87496900	2.64993800	3.30546200
C	-4.05522700	0.32108800	4.82447900
H	-3.34427200	-0.70858500	3.07422400
C	-4.30030400	2.71181000	4.62985700
H	-3.80298500	3.56981900	2.72487000
C	-4.38867300	1.54963600	5.39002200
H	-4.12581800	-0.59376600	5.41066600
H	-4.56497200	3.67275400	5.06806300
H	-4.71817700	1.60182600	6.42607400
C	-3.31219200	-3.13955600	1.49167800
C	-4.61524600	-2.72005700	1.18438200
C	-3.04749100	-3.61497500	2.78100600
C	-5.62359300	-2.78926500	2.13822800
H	-4.84453300	-2.32892000	0.19166800

C	-4.06025100	-3.68197500	3.73460700
H	-2.04563800	-3.94408100	3.05554800
C	-5.35013200	-3.26893400	3.41693600
H	-6.62887400	-2.46177200	1.87784500
H	-3.83839500	-4.06706100	4.72872200
H	-6.14143300	-3.32230200	4.16249200
C	-2.57229400	-3.31642700	-1.31964600
C	-3.47200100	-4.37493500	-1.47965200
C	-2.08618800	-2.65008600	-2.45031200
C	-3.88859400	-4.75238600	-2.75113700
H	-3.85369400	-4.89991400	-0.60328000
C	-2.49322500	-3.04135100	-3.72266100
H	-1.36728600	-1.83355900	-2.33408200
C	-3.40098200	-4.08568000	-3.87285400
H	-4.59347800	-5.57369200	-2.86887000
H	-2.09506900	-2.52999000	-4.59791100
H	-3.72462400	-4.38820500	-4.86729500
C	2.13019500	-4.67691300	0.77213600
C	2.82416500	-5.79765900	0.31476000
C	2.41512900	-4.16948400	2.04780700
C	3.76914600	-6.41628700	1.13136100
H	2.62729700	-6.19514000	-0.68053800
C	3.34536900	-4.79752600	2.86373700
H	1.91866500	-3.26136000	2.39874800
C	4.02444900	-5.92502100	2.40637300
H	4.30189200	-7.29288900	0.76628100
H	3.56456000	-4.38757400	3.84849900
H	4.76297100	-6.41196600	3.04134100
C	0.71846500	-4.67979900	-1.78776900
C	0.17231700	-5.96730100	-1.83686300
C	1.12999000	-4.06687500	-2.97441800
C	0.04794100	-6.62998100	-3.05171500
H	-0.14240300	-6.46702700	-0.91935300
C	1.00453100	-4.73085500	-4.19085400
H	1.53584300	-3.05364300	-2.93885300
C	0.46292100	-6.01096500	-4.22916000
H	-0.37579700	-7.63219700	-3.08146100
H	1.32665400	-4.24456300	-5.11001000
H	0.36272800	-6.53257900	-5.17943500
C	4.83351800	0.55945700	-0.80260600
C	6.01600800	1.19574600	-0.40995200
C	4.51761300	0.47094800	-2.16004200
C	6.86752400	1.73836500	-1.36300400
H	6.27990400	1.25424900	0.64754600
C	5.37701200	1.00870600	-3.11638600
H	3.59015500	-0.02179600	-2.45995100
C	6.55006200	1.64022700	-2.71707100
H	7.78494700	2.23494900	-1.05187400
H	5.13153000	0.92780700	-4.17410000
H	7.22491000	2.05603000	-3.46346400
C	4.78662900	-1.20730200	1.45325300
C	5.29749000	-2.36377600	0.84969800
C	5.10600900	-0.93761400	2.78507700
C	6.14158300	-3.21176900	1.55151800
H	5.02658500	-2.60020400	-0.18201600
C	5.93838000	-1.80187300	3.49493700

H	4.71481000	-0.04933400	3.28061400
C	6.46298000	-2.93197600	2.87851300
H	6.53655800	-4.10387300	1.06848200
H	6.18465100	-1.58115700	4.53231500
H	7.12029200	-3.60035200	3.43236600

L^{ph}

E(M06/BS1) = -1647.753043 au

H(M06/BS1) = -1647.335460 au

G(M06/BS1) = -1647.415099 au

E(M06/BS2//M06/BS1) = -1648.173935 au

E(B3LYP-D3BJ/BS2//M06/BS1) = -1649.152524 au

C	-0.15652900	-1.16618900	-0.32843300
H	-0.01965600	-1.01525600	0.75308800
H	-0.48718000	-2.20281600	-0.48187100
P	1.43122900	-0.93731700	-1.28097900
P	-1.50014200	-0.04756900	-1.01543400
C	-2.98624000	-1.00570700	-0.47638100
C	-4.00413700	-0.48090800	0.32459500
C	-3.15925000	-2.28838500	-1.01298600
C	-5.14361200	-1.22983100	0.60828400
H	-3.90657600	0.52216100	0.73803000
C	-4.29163200	-3.03932300	-0.72442100
H	-2.40075400	-2.70524100	-1.67893700
C	-5.28857200	-2.51225400	0.09249000
H	-5.92152400	-0.80484000	1.24132800
H	-4.40090100	-4.03758600	-1.14615000
H	-6.17811700	-3.09761400	0.31961700
C	-1.45242200	1.33328800	0.20555700
C	-1.45638600	1.14268200	1.59304100
C	-1.37363700	2.63548700	-0.29091500
C	-1.37620600	2.22620600	2.45821800
H	-1.53502800	0.13415500	2.00205000
C	-1.29088500	3.72456100	0.57368100
H	-1.35673300	2.79521600	-1.36977700
C	-1.29037300	3.52070000	1.94809300
H	-1.38207900	2.06334000	3.53517100
H	-1.21822400	4.73296000	0.16837600
H	-1.22481400	4.37010700	2.62661500
C	1.75308500	0.84945900	-0.94751900
C	1.97206100	1.36079600	0.33703300
C	1.72792000	1.73045000	-2.03084300
C	2.14983300	2.72362300	0.53239100
H	1.99669900	0.68192100	1.19117300
C	1.91429400	3.09792600	-1.83844100
H	1.55606700	1.33501700	-3.03289200
C	2.12342100	3.59361500	-0.55697600
H	2.29994500	3.11411700	1.53818800
H	1.89692700	3.77409700	-2.69206600
H	2.26492300	4.66265300	-0.40220800
C	2.64746700	-1.71013800	-0.13113300
C	3.99979500	-1.36830800	-0.26749900
C	2.30296500	-2.69393400	0.79988700
C	4.97222000	-1.97690400	0.51449300

H	4.29113500	-0.60439300	-0.99028900
C	3.27865400	-3.30929600	1.58109100
H	1.26168800	-2.98994100	0.92542700
C	4.61432500	-2.95157100	1.44366300
H	6.01645700	-1.68974300	0.39916900
H	2.98827000	-4.07056100	2.30402000
H	5.37623700	-3.43074400	2.05631200

$[Ag_3(H)(BH_4)L^{Ph}]^+$

E(M06/BS1) = -2112.843086 au

H(M06/BS1) = -2112.366417 au

G(M06/BS1) = -2112.471802 au

E(M06/BS2//M06/BS1) = -2117.045602 au

C	1.19804900	0.72864200	-1.23993400
H	2.09599000	1.36379400	-1.27561200
H	0.90555200	0.48283300	-2.27061100
B	-4.56184100	-0.45392400	-0.73297900
H	-4.23791100	0.23551400	0.25873100
H	-5.61405600	-0.01354000	-1.10526500
H	-1.84636300	-2.74206500	1.43493400
Ag	-2.34489000	0.51184800	-0.68289100
P	-0.20280200	1.65297600	-0.46555200
P	1.55043800	-0.87179200	-0.37385400
H	-3.79336000	-0.44366400	-1.72539700
H	-4.83131400	-1.65514200	-0.44645100
Ag	-0.47539800	-1.86546000	0.61458000
Ag	-3.28976100	-2.11208100	0.58705300
C	0.28827200	1.89051100	1.26738700
C	1.47473100	2.56566000	1.58107700
C	-0.50642600	1.37191400	2.29368500
C	1.87011700	2.69274000	2.90493600
H	2.08899800	2.99382900	0.78741500
C	-0.11047400	1.50800700	3.62199200
H	-1.44634100	0.86707900	2.05576300
C	1.07978000	2.16076500	3.92380600
H	2.79612700	3.21085300	3.14647100
H	-0.73693600	1.11087100	4.41790800
H	1.39053300	2.26807900	4.96131500
C	-0.15267500	3.30395500	-1.22482800
C	0.40281100	3.52785100	-2.48725200
C	-0.77452500	4.35583600	-0.54204500
C	0.34737200	4.79771900	-3.05331600
H	0.88247400	2.72074600	-3.04008800
C	-0.82653500	5.62030100	-1.11331500
H	-1.21144400	4.18867000	0.44367800
C	-0.26547100	5.84176700	-2.36893000
H	0.78568300	4.96923100	-4.03431100
H	-1.30771700	6.43586000	-0.57770200
H	-0.30947900	6.83246700	-2.81630500
C	2.82253700	-0.48003700	0.86604700
C	4.04383700	0.09336500	0.49337700
C	2.57789700	-0.77303400	2.20889600
C	4.99762000	0.38522400	1.45912300
H	4.26251300	0.29657300	-0.55597600

C	3.53635200	-0.48097400	3.17472200
H	1.62779800	-1.22159100	2.50685300
C	4.74261000	0.09994800	2.79984600
H	5.94828500	0.82599800	1.16597200
H	3.33820800	-0.71019900	4.21999200
H	5.49525100	0.32279600	3.55358500
C	2.34645500	-1.90127900	-1.64159300
C	2.20743200	-3.28853200	-1.53108000
C	3.11602400	-1.36532100	-2.68012000
C	2.83545500	-4.13024100	-2.44193500
H	1.60281900	-3.71385200	-0.72769100
C	3.73639200	-2.20997400	-3.59281400
H	3.23402800	-0.28670200	-2.78721100
C	3.59774300	-3.59036100	-3.47302800
H	2.72187900	-5.20821600	-2.35079300
H	4.33040500	-1.78925100	-4.40145700
H	4.08304800	-4.24827100	-4.19081000

$[Ag_3(H)_2L^{Ph}{}_2]^+$

E(M06/BS1) = -3734.032094 au

H(M06/BS1) = -3733.170615 au

G(M06/BS1) = -3733.326060 au

E(M06/BS2//M06/BS1) = -3738.636247 au

C	-3.70899500	0.17538600	-0.68329400
H	-4.59355000	0.59071100	-0.17550400
H	-3.96686000	0.04274600	-1.74521000
H	0.56395700	-3.26033400	-0.42095000
Ag	-1.02965100	-2.41577900	-0.50901000
P	-3.29492100	-1.51973400	-0.05145700
P	-2.31179300	1.39979600	-0.72520000
H	0.55303800	-0.79072300	-2.64175000
C	3.53231000	0.87882500	-0.47531700
H	4.33186400	1.38015500	0.09111600
H	3.58885700	1.22873000	-1.51816200
Ag	-0.09794200	0.38924600	-1.37299300
P	1.84534600	1.39490200	0.11074700
P	3.75083500	-0.96603200	-0.52743900
Ag	1.57695200	-1.91989600	-1.40009100
C	-2.92090900	2.62752600	-1.92777400
C	-3.95780900	3.51188300	-1.61259300
C	-2.34559200	2.65709000	-3.20110200
C	-4.41662600	4.41107300	-2.56669900
H	-4.39623200	3.50345800	-0.61348100
C	-2.80891600	3.55901000	-4.15467500
H	-1.53559500	1.96598700	-3.44671700
C	-3.84246900	4.43375400	-3.83664400
H	-5.22284000	5.09939200	-2.32047300
H	-2.35989100	3.57930100	-5.14578800
H	-4.20362100	5.14105600	-4.58087100
C	-2.32625300	2.29038000	0.86679100
C	-3.07817500	1.90800600	1.97809100
C	-1.44615900	3.37713100	0.97727900
C	-2.93415600	2.58239200	3.18925000
H	-3.77880100	1.07718900	1.92138000

C	-1.32145200	4.05945000	2.17907600
H	-0.85234700	3.68993200	0.11446100
C	-2.05683900	3.65506700	3.29244100
H	-3.51811400	2.26033000	4.05044200
H	-0.63816600	4.90418800	2.24738200
H	-1.94631200	4.18079500	4.23897000
C	-4.63231600	-2.57991000	-0.68958100
C	-4.40009900	-3.95973700	-0.66929100
C	-5.85837800	-2.09721200	-1.15674300
C	-5.38173400	-4.84372600	-1.09879900
H	-3.44180300	-4.34445700	-0.31334300
C	-6.83567600	-2.98539600	-1.59485900
H	-6.06333200	-1.02706400	-1.18409600
C	-6.59966000	-4.35592300	-1.56443800
H	-5.19138600	-5.91477600	-1.07994100
H	-7.78588000	-2.60283400	-1.96241300
H	-7.36542900	-5.04708300	-1.91069500
C	-3.59345000	-1.43472000	1.74780900
C	-4.89003600	-1.30131100	2.25717600
C	-2.50565900	-1.44887000	2.62433300
C	-5.09102300	-1.15258300	3.62388700
H	-5.74707500	-1.31978300	1.58221400
C	-2.71132100	-1.31137500	3.99450000
H	-1.49139500	-1.56889400	2.23432000
C	-4.00052100	-1.15437500	4.49249800
H	-6.10052700	-1.04789200	4.01661400
H	-1.86107700	-1.34080300	4.67419300
H	-4.16063100	-1.04962200	5.56397000
C	1.89590100	3.20592200	-0.16117100
C	2.08756900	4.13749900	0.86065900
C	1.63950300	3.65807200	-1.46254200
C	2.02648600	5.50070700	0.58319400
H	2.26581500	3.79919200	1.88146800
C	1.58498600	5.01907300	-1.73813300
H	1.47146200	2.93420400	-2.26535100
C	1.77350300	5.94248700	-0.71168900
H	2.17635600	6.22254800	1.38456500
H	1.38676800	5.36068000	-2.75237000
H	1.72200700	7.00871300	-0.92335800
C	1.85373400	1.18200300	1.92219500
C	2.98335600	1.37902100	2.72398600
C	0.64237400	0.83605100	2.52884700
C	2.89965800	1.23120700	4.10335300
H	3.94180800	1.64282800	2.27639700
C	0.55370800	0.70956600	3.91131700
H	-0.24686500	0.67596300	1.91427700
C	1.68408800	0.90141600	4.69907700
H	3.78658300	1.37942900	4.71654400
H	-0.40768500	0.47349000	4.36657400
H	1.62015000	0.79741000	5.78071300
C	5.28921600	-1.20082400	-1.47630100
C	5.48582600	-2.45819600	-2.05764400
C	6.26337100	-0.21125800	-1.63940000
C	6.64376700	-2.72701200	-2.77725900
H	4.72290000	-3.23070700	-1.94440900
C	7.41794300	-0.48037600	-2.36718100

H	6.12754700	0.77709700	-1.19986700
C	7.60931300	-1.73674700	-2.93380300
H	6.78812000	-3.70839200	-3.22485100
H	8.17090200	0.29542600	-2.49316500
H	8.51276600	-1.94417100	-3.50393500
C	4.17722500	-1.38641300	1.20016200
C	5.44380900	-1.12580600	1.73242800
C	3.18872100	-1.94683100	2.01380300
C	5.71328700	-1.41342500	3.06538600
H	6.22846300	-0.71053700	1.09806500
C	3.45895500	-2.22570300	3.34966200
H	2.20106000	-2.15874500	1.59723200
C	4.72052900	-1.96294700	3.87406900
H	6.70418800	-1.22017900	3.47259000
H	2.68342900	-2.65742300	3.97994900
H	4.93602200	-2.19428100	4.91589800

$[Ag_3(H)_2L^{Ph}]^+$

E(M06/BS1) = -2086.21344 au

H(M06/BS1) = -2085.773971 au

G(M06/BS1) = -2085.871002 au

E(M06/BS2//M06/BS1) = -2090.401324 au

C	-1.12363400	0.17555400	1.31058300
H	-2.19262400	0.37700400	1.47610700
H	-0.66135700	0.00238500	2.29231300
H	2.94677600	-1.92045100	-1.44646500
Ag	2.15296200	1.44178600	0.51499900
P	-0.30849100	1.64206700	0.52958900
P	-0.93478900	-1.39337500	0.32988400
H	3.94983000	1.11588900	0.28373000
Ag	1.25822100	-1.65536900	-0.77041100
Ag	3.77694700	-0.47231100	-0.65781100
C	-0.96337100	1.66486900	-1.16827500
C	-2.33068500	1.85011300	-1.40797400
C	-0.09777800	1.43853200	-2.24221100
C	-2.82199400	1.79082400	-2.70495100
H	-3.01205100	2.04298000	-0.57803700
C	-0.59274200	1.38382900	-3.54263100
H	0.97264400	1.31087000	-2.06240700
C	-1.95409000	1.55497400	-3.77066100
H	-3.88660500	1.92577800	-2.88692800
H	0.08723600	1.21704200	-4.37551000
H	-2.34279900	1.51486400	-4.78656900
C	-1.03691100	3.08528000	1.36218800
C	-0.93352300	4.32706700	0.72326200
C	-1.61120900	3.00634800	2.63322800
C	-1.41577200	5.47104600	1.34472800
H	-0.48509500	4.39846800	-0.26893100
C	-2.09093700	4.15757900	3.25126100
H	-1.69009300	2.05299300	3.15484200
C	-1.99525400	5.38693200	2.60878600
H	-1.33873300	6.43254500	0.84138500
H	-2.54150900	4.09005300	4.23932500
H	-2.37136200	6.28488300	3.09454800

C	-1.11500700	-2.67665500	1.61130200
C	-2.16523000	-3.59553800	1.62751100
C	-0.10049800	-2.76437300	2.57343900
C	-2.20754300	-4.58011600	2.61146900
H	-2.94934600	-3.54919600	0.87310900
C	-0.15353800	-3.74153300	3.55786100
H	0.74398900	-2.06967800	2.54884600
C	-1.20948300	-4.65093400	3.57651500
H	-3.02764600	-5.29506600	2.62101700
H	0.63503800	-3.80310100	4.30492700
H	-1.24776600	-5.42212600	4.34291700
C	-2.39430800	-1.45878500	-0.74610000
C	-3.68835100	-1.25525700	-0.24852200
C	-2.21218200	-1.71260700	-2.10683700
C	-4.77965700	-1.30377200	-1.10598600
H	-3.84922400	-1.07356200	0.81544900
C	-3.30735800	-1.75849100	-2.96400800
H	-1.20724900	-1.86586700	-2.50359100
C	-4.58876600	-1.55499800	-2.46399300
H	-5.78327500	-1.15238200	-0.71358100
H	-3.15652800	-1.95291900	-4.02403800
H	-5.44620900	-1.59407800	-3.13295600