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Supporting Information

Metal–Ligand Cooperativity of the Calix[4]pyrrolato Aluminate: Triggerable C–C Bond Formation and Rate Control in Catalysis

*Fabian Ebner, Lukas Maximilian Sigmund, and Lutz Greb**

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1. Materials and Methods

Unless otherwise stated, all manipulations were carried out under a dry argon atmosphere by using standard Schlenk techniques to prevent oxidation and hydrolysis of sensitive compounds. All solvents were rigorously dried by applying standard procedures, freshly degassed and stored over molecular sieve (3 Å resp. 4 Å) before use. All glassware, syringes, magnetic stirring bars, and needles were thoroughly dried. The commercially available chemicals were used as received. Lithium aluminum hydride was purified by dissolving in dry ether followed by filtration and evaporation of the solvent. All air-sensitive compounds were stored in a glove box (MBraun LABmaster dp, MB-20-G or Sylatech Glovebox) under N_2 atmosphere. The purity and identity of the compounds were confirmed by high-resolution multinuclear NMR spectroscopy, mass spectrometry, and if possible, X-ray diffraction analysis. ^{1}H, ^{7}Li, and $^{13}C\{^{1}H\}$ NMR spectra were collected with a Bruker DPX 200, Bruker Advance II 400 or Bruker 2 Advance III 600 NMR spectrometer and referenced to the solvent in use. Chemical shifts are reported as dimensionless δ values in ppm, coupling constants J are given in hertz (Hz). Electrospray ionization mass spectra were obtained with a Bruker ApexQe FT-ICR instrument. IR-Spectra was recorded on a BIORAD Excalibur FTS 3000 Spectrometer and processed with BioRad Merlin and OriginPro 2017G 64Bit. All KBr pellets were prepared under a nitrogen atmosphere in a glovebox and measured immediately after exposure to air. *meso*-Octamethylcalix[4]pyrrole (CX) was prepared from acetone and pyrrole according to the literature and purified via flash column chromatography.[1]

2. Synthesis

Synthesis of [Li(thf)$_4$][**1***-CO_2]:

A solution of [Li(thf)$_4$][**1**-thf] (100 mg, 122 µmol) in tetrahydrofuran was subjected toward carbon dioxide (2 bar) and quantitative conversion was observed after 12 h at room temperature. The analog reaction in dichloromethane as solvent showed full conversion in minutes after addition of carbon dioxide, as detected by ^{1}H NMR spectroscopy. All volatiles were removed under reduced pressure and a yellow solid was obtained. Yield: 97% (93 mg, 117 µmol). ^{1}H NMR (THF-d_8, 400 MHz, 295 K) δ[ppm]: 7.69 (d, $^3J_{HH}$ = 5.0 Hz, 1H, *H2*), 6.86 (d, $^3J_{HH}$ = 5.0 Hz, 1H, *H3*), 5.82 (d, $^3J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 5.76 (d, $^3J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 5.73 (d, $^3J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 5.68 (m, 3H, $H_{pyrrole}$), 3.61 (m, 16H, H_{THF1}), 1.77 (m, 16H, H_{THF1}), 1.75 (s, 3H, H_{CH3}), 1.74 (s, 3H, H_{CH3}), 1.71 (s, 3H, H_{CH3}), 1.62 (s, 3H, H_{CH3}), 1.60 (s, 3H, H_{CH3}), 1.38 (s, 3H, H_{CH3}), 1.33 (s, 3H, H_{CH3}), 0.92 (s, 3H, H_{CH3}). ^{13}C{^{1}H} {^{1}H} NMR (THF-d_8, 100 MHz, 295 K) δ[ppm]: 188.3 (*C4*), 173.1 (C_{CO2}/*C5*), 156.7 (*C2*), 150.9 ($C_{q,pyrrole}$), 149.8 ($C_{q,pyrrole}$), 147.0 ($C_{q,pyrrole}$), 146.7 ($C_{q,pyrrole}$), 144.7 ($C_{q,pyrrole}$), 140.3 ($C_{q,pyrrole}$), 128.5 (*C3*), 104.1 ($C_{CH,pyrrole}$), 103.4 ($C_{CH,pyrrole}$), 102.2 ($C_{CH,pyrrole}$), 101.8 ($C_{CH,pyrrole}$), 101.5 ($C_{CH,pyrrole}$), 100.8 ($C_{CH,pyrrole}$), 97.3 (*C1*), 68.0 (C_{THF}), 44.9 (C_q), 40.9 (C_{CH3}), 39.2 (C_q), 36.8 (C_{CH3}), 36.7 (C_q), 36.7 (C_q), 36.6 (C_{CH3}), 28.4 (C_{CH3}), 27.4 (C_{CH3}), 27.3 (C_{CH3}), 26.7 (C_{CH3}), 24.0 (C_{CH3}). ^{7}Li NMR (THF-d_8, 155 MHz, 295 K) δ[ppm]: -0.5. [HR-ESI$^-$]: calc: 495.2340 m/z ([**1***-CO_2]$^-$) exp. 495.2332 m/z ([**1***-CO_2]$^-$). IR (KBr): C=O band at $\tilde{\nu}$ = 1665 cm^{-1}.

Synthesis of [PPh_4][**1***-CO_2]:

A solution of [PPh_4][**1**] (100 mg, 126 µmol, 1.00 eq.) in 3 ml dichloromethane was subjected toward carbon dioxide (2 bar) and quantitative conversion was observed immediately at room temperature by ^{1}H NMR spectroscopy. All volatiles were removed under reduced pressure and a yellow solid was obtained. The CO_2 adduct is persistent at room temperature, and no CO_2 release is observed upon heating under vacuum. Suitable crystals for SCXRD were obtained from a 1:1 mixture of dichloromethane/toluene at room temperature. ^{1}H NMR (DCM-d_2, 600 MHz, 295 K) δ[ppm]: 7.84 (m, 4H, PPh_4^+), 7.67-7.65 (m, 8H, PPh_4^+), 7.65 (d, $^3J_{HH}$ = 5.0 Hz, 1H, *H2*), 7.56-7.54 (m, 8H, PPh_4^+), 6.68 (d, $^3J_{HH}$ = 5.0 Hz, 1H, *H3*), 5.90 (d, $^3J_{HH}$ = 2.8 Hz, 1H, $H_{pyrrole}$), 5.86 (d, $^3J_{HH}$ = 2.9 Hz, 2H, $H_{pyrrole}$), 5.81 (d, $^3J_{HH}$ = 2.9 Hz, 2H, $H_{pyrrole}$) 5.77 (d, $^3J_{HH}$ = 2.9 Hz, 1H, $H_{pyrrole}$), 5.75 (d, $^3J_{HH}$ = 2.9 Hz, 1H, $H_{pyrrole}$), 5.73 (d, $^3J_{HH}$ = 2.9 Hz, 1H, $H_{pyrrole}$), 1.75 (s, 3H, H_{CH3}), 1.75 (s, 3H, H_{CH3}) 1.68 (s, 3H, H_{CH3}), 1.64 (s, 3H, H_{CH3}), 1.58 (s, 3H, H_{CH3}), 1.40 (s, 3H, H_{CH3}), 1.36 (s, 3H, H_{CH3}), 0.92 (s, 3H, H_{CH3}). ^{13}C{^{1}H} NMR (DCM-d_2, 150 MHz, 295 K) δ[ppm]: 186.9 (C_q *C4*, identified by ^{1}H/^{13}C{^{1}H} HMBC NMR), 166.87 (C_{CO2}/*C5*), 158.1 (*C2*), 150.4 ($C_{q,pyrrole}$), 148.7 ($C_{q,pyrrole}$), 147.5 ($C_{q,pyrrole}$), 146.9 ($C_{q,pyrrole}$), 146.3 ($C_{q,pyrrole}$), 141.7 ($C_{q,pyrrole}$), 136.2 (d, $^4J_{CP}$ = 3.1 Hz, CH, PPh_4^+), 134.8 (d, $^2J_{CP}$ = 10.3 Hz, CH, PPh_4^+), 131.0 (d, $^3J_{CP}$ = 12.9 Hz, CH, PPh_4^+), 127.1 (CH, *C3*), 117.9 (d, $^1J_{CP}$ = 89.8 Hz, C_q , PPh_4^+), 103.7 ($C_{CH,pyrrole}$), 102.6 ($C_{CH,pyrrole}$), 102.0 ($C_{CH,pyrrole}$), 101.8 ($C_{CH,pyrrole}$), 101.5 ($C_{CH,pyrrole}$), 100.2 ($C_{CH,pyrrole}$), 97.9 (*C1*), 44.3 (C_q), 41.5 (C_{CH3}), 38.8 (C_q), 36.5 (C_{CH3}), 36.4 (C_q), 36.3 (C_q), 35.4 (C_{CH3}), 28.1 (C_{CH3}), 27.7 (C_{CH3}), 27.3 (C_{CH3}), 26.4 (C_{CH3}), 24.0 (C_{CH3}). ^{31}P NMR (DCM-d_2, 243 MHz, 295 K) δ[ppm]: 23.18.

Synthesis of [PPh_4][**1***-cyclohexanecarboxaldehyde]:

To a solution of [PPh_4][**1**] (100 mg, 126 µmol, 1.00 eq.) in 3 ml dichloromethane cyclohexanecarboxaldehyde (16.9 mg, 151 µmol, 1.20 eq.) was added and stirred for 5 min. Full conversion was detected by ^{1}H NMR spectroscopy. 4 ml *n*-pentane was added to the solution, the solution cooled to -40 °C for 30 min and the yellowish solid was separated by filtration from the solution. The solid was again dissolved in 3 ml dichloromethane and precipitated again with 4 ml *n*-pentane, separated by filtration and dried *in vacuo* to obtain [PPh_4][**1***-cyclohexanecarboxaldehyde] as yellow solid. Suitable crystals for SCXRD were obtained from a 1:1 mixture of dichloromethane/toluene at room temperature. ^{1}H NMR (DCM-d_2, 400 MHz, 295 K) δ[ppm]: 7.87 (m, 4H, PPh_4^+), 7.72-7.68 (m, 8H, PPh_4^+), 7.64 (d, $^3J_{HH}$ = 5.0 Hz, 1H, *H2*), 7.59-7.56 (m, 8H, PPh_4^+), 6.63 (d, $^3J_{HH}$ = 5.0 Hz, 1H, *H3*), 5.89 (d, $^3J_{HH}$ = 2.8 Hz, 1H, $H_{pyrrole}$), 5.78 (d, $^3J_{HH}$ = 2.9 Hz, 2H, $H_{pyrrole}$), 5.77 (d, $^3J_{HH}$ = 2.9 Hz, 2H, $H_{pyrrole}$) 5.69 (d, $^3J_{HH}$ = 2.9 Hz, 1H, $H_{pyrrole}$), 5.67 (d, $^3J_{HH}$ = 2.9 Hz, 1H, $H_{pyrrole}$), 5.64 (d, $^3J_{HH}$ = 2.9 Hz, 1H, $H_{pyrrole}$), 4.14 (d, $^3J_{HH}$ = 4.2 Hz, 1H,

H$_{Aldehyd}$), 1.72 (s, 3H, *H*$_{CH3}$), 1.62 (s, 3H, *H*$_{CH3}$), 1.61 (s, 9H, *H*$_{CH3}$), 1.56 (s, 3H, *H*$_{CH3}$), 1.54 (m, 1H, *H*$_{Cyhex}$), 1.48 (m, 1H, *H*$_{Cyhex}$), 1.41 (m, 1H, *H*$_{Cyhex}$), 1.36 (m, 1H, *H*$_{Cyhex}$), 1.29 (m, 1H, *H*$_{Cyhex}$), 1.26 (m, 1H, *H*$_{Cyhex}$), 1.17 (m, 1H, *H*$_{Cyhex}$), 1.10 (m, 1H, *H*$_{Cyhex}$), 1.02 (m, 1H, *H*$_{Cyhex}$), 0.78 (s, 3H, *H*$_{CH3}$), 0.71 (m, 1H, *H*$_{Cyhex}$). $^{13}C\{^1H\}$ NMR (DCM-*d*$_2$, 100 MHz, 295 K) δ[ppm]: 183.4 (C_q *C4*, identified by $^1H/^{13}C\{^1H\}$ HMBC NMR), 160.3 (CH, *C2*), 150.2 (C_q, *C*$_{pyrrole}$), 148.7 (C_q, *C*$_{pyrrole}$), 147.4 (C_q, *C*$_{pyrrole}$), 147.4 (C_q, *C*$_{pyrrole}$), 147.0 (C_q, *C6*), 141.7 (C_q, *C*$_{pyrrole}$), 136.2 (d, $^4J_{CP}$ = 3.1 Hz, CH, *PPh*$_4^+$), 134.8 (d, $^2J_{CP}$ = 10.3 Hz, CH, *PPh*$_4^+$), 131.0 (d, $^3J_{CP}$ = 12.9 Hz, CH, *PPh*$_4^+$), 126.9 (CH, *C3*), 117.9 (d, $^1J_{CP}$ = 89.8 Hz, C_q , *PPh*$_4^+$), 103.0 (CH, *C*$_{pyrrole}$), 101.0 (CH, *C*$_{pyrrole}$), 100.8 (CH, *C*$_{pyrrole}$), 100.7 (CH, *C*$_{pyrrole}$), 100.4 (CH, *C*$_{pyrrole}$), 98.9 (CH, *C*$_{pyrrole}$), 96.8 (C_q, *C1*), 81.3 (CH, *C5*), 46.8 (*C*$_{CH3}$), 44.8 (*C*$_q$), 41.5 (*C*$_{CH3}$), 38.7 (*C*$_q$), 36.6 (*C*$_q$), 36.5 (*C*$_{CH3}$), 36.5 (*C*$_q$), 35.8 (*C*$_{CH3}$), 34.5 (*C*$_q$), 32.5 (*C*$_{CH2}$), 28.2 (*C*$_{CH3}$), 27.8 (*C*$_{CH3}$), 27.4 (*C*$_{CH2}$), 27.3 (*C*$_{CH3}$), 27.2 (*C*$_{CH2}$), 26.9 (*C*$_{CH2}$), 26.7 (*C*$_{CH3}$), 26.1 (*C*$_{CH2}$), 24.3 (*C*$_{CH3}$). ^{31}P NMR (DCM-*d*$_2$, 243 MHz, 295 K) δ[ppm]: 23.24.

Synthesis of [PPh_4][**1***-*p*-nitrobenzaldehyde]:

To a solution of [PPh_4][**1**] (100 mg, 126 µmol, 1.00 eq.) in 3 ml dichloromethane *p*-nitrobenzaldehyde (22.8 mg, 151 µmol, 1.20 eq.) was added and stirred for 5 min. Full conversion was detected *via* ^1H NMR spectroscopy. 4 ml *n*-pentane were added to the solution and the reddish solid was separated by filtration from the solution. The solid was again dissolved in 2 ml dichloromethane and precipitated again with 4 ml *n*-pentane, separated by filtration and dried *in vacuo* to obtain [PPh_4][**1***-*p*-nitrobenzaldehyde] as red solid. Suitable crystals for SCXRD were obtained from dichloromethane at room temperature. ^1H NMR (DCM-*d*$_2$, 600 MHz, 295 K) δ[ppm]: 7.90-7.86 (m, 4H, *PPh*$_4^+$), 7.75 (d, $^3J_{HH}$ = 8.6 Hz, 2H, *H8*), 7.73-7.68 (m, 8H, *PPh*$_4^+$), 7.60-7.54 (m, 8H, *PPh*$_4^+$), 6.91 (d, $^3J_{HH}$ = 5.2 Hz, 1H, *H2*), 6.74 (d, $^3J_{HH}$ = 8.6 Hz, 2H, *H7*), 6.06 (d, $^3J_{HH}$ = 5.1 Hz, 1H, *H3*), 6.01 (d, $^3J_{HH}$ = 2.9 Hz, 1H, *H*$_{pyrrole}$), 5.92 (d, $^3J_{HH}$ = 2.9 Hz, 1H, *H*$_{pyrrole}$), 5.85 (d, $^3J_{HH}$ = 3.1 Hz, 1H, *H*$_{pyrrole}$), 5.84 (d, $^3J_{HH}$ = 3.1 Hz, 1H, *H*$_{pyrrole}$), 5.73 (d, $^3J_{HH}$ = 2.8 Hz, 1H, *H*$_{pyrrole}$), 5.70 (d, $^3J_{HH}$ = 2.8 Hz, 1H, *H*$_{pyrrole}$), 5.62 (s, 1H, *H5*), 1.87 (s, 3H, *H*$_{CH3}$), 1.68 (s, 3H, *H*$_{CH3}$), 1.67 (s, 3H, *H*$_{CH3}$), 1.62 (s, 3H, *H*$_{CH3}$), 1.62 (s, 3H, *H*$_{CH3}$), 1.54 (s, 3H, *H*$_{CH3}$), 1.40 (s, 3H, *H*$_{CH3}$), 0.87 (s, 3H, *H*$_{CH3}$). $^{13}C\{^1H\}$ NMR (DCM-*d*$_2$, 150 MHz, 295 K) δ[ppm]: 187.6 (C_q *C4*, identified by $^1H/^{13}C\{^1H\}$ HMBC NMR), 160.7 (CH, *C2*), 150.8 (C_q, *C*$_{pyrrole}$), 148.9 (C_q, *C*$_{pyrrole}$), 147.1 (C_q, *C*$_{pyrrole}$), 146.8 (C_q, *C*$_{pyrrole}$), 146.47 (C_q, *C6*), 146.4 (C_q, *C*$_{pyrrole}$) 141.6 (C_q, *C*$_{pyrrole}$), 136.2 (d, $^4J_{CP}$ = 3.1 Hz, CH, *PPh*$_4^+$), 134.8 (d, $^2J_{CP}$ = 10.3 Hz, CH, *PPh*$_4^+$), 131.0 (d, $^3J_{CP}$ = 12.9 Hz, CH, *PPh*$_4^+$), 127.2 (CH, *C7*), 124.9 (CH, *C3*), 123.1 (CH, *C8*), 117.9 (d, $^1J_{CP}$ = 89.8 Hz, C_q, *PPh*$_4^+$), 103.3 (CH, *C*$_{pyrrole}$), 102.6 (CH, *C*$_{pyrrole}$), 101.3 (CH, *C*$_{pyrrole}$), 101.1 (CH, *C*$_{pyrrole}$), 100.9 (CH, *C*$_{pyrrole}$), 99.1 (CH, *C*$_{pyrrole}$), 96.2 (C_q, *C1*), 77.9 (CH, *C5*), 42.9 (*C*$_q$), 41.0 (*C*$_q$), 38.8 (*C*$_q$), 36.7 (*C*$_q$), 36.6 (*C*$_{CH3}$), 36.1 (*C*$_{CH3}$), 35.8 (*C*$_{CH3}$), 29.5 (*C*$_{CH3}$), 28.5 (*C*$_{CH3}$), 27.1 (C_{CH3}), 26.6 (*C*$_{CH3}$), 24.1 (*C*$_{CH3}$). ^{31}P NMR (DCM-*d*$_2$, 243 MHz, 295 K) δ[ppm]: 23.25.

Synthesis of [PPh_4][**1***-*p*-methylbenzaldehyde]:

To a solution of [PPh_4][**1**] (100 mg, 122 µmol, 1.00 eq.) in 3 ml dichloromethane *p*-methylbenzaldehyde (18.1 mg, 151 µmol, 1.20 eq.) was added and stirred for 5 min. Full conversion was proved by ^1H NMR spectroscopy. Crystallization started immediately at rt and after 24 h at rt the crystals were separated by filtration to obtain [PPh_4][**1***-*p*-methylbenzaldehyde] as yellow crystals. These were also suitable for SCXRD. For obtaining the product, the reaction mixture can be immediately treated after mixing with 6 ml *n*-pentane. The solid was separated by filtration and washed three times with 6 ml *n*-pentane. ^1H NMR (DCM-*d*$_2$, 600 MHz, 295 K) δ[ppm]: 7.85 (m, 4H, *PPh*$_4^+$), 7.67 (m, 8H, *PPh*$_4^+$), 7.56-7.54 (m, 8H, *PPh*$_4^+$), 6.94 (d, $^3J_{HH}$ = 5.2 Hz, 1H, *H2*), 6.72 (d, $^3J_{HH}$ = 7.7 Hz, 2H, *H7*), 6.06 (d, $^3J_{HH}$ = 7.7 Hz, 1H, *H3*), 6.08 (d, $^3J_{HH}$ = 5.2 Hz, 1H, *H*$_{pyrrole}$), 5.98 (d, $^3J_{HH}$ = 2.9 Hz, 1H, *H*$_{pyrrole}$), 5.87 (d, $^3J_{HH}$ = 3.1 Hz, 1H, *H*$_{pyrrole}$), 5.82 (d, $^3J_{HH}$ = 3.1 Hz, 1H, *H*$_{pyrrole}$), 5.79 (d, $^3J_{HH}$ = 2.8 Hz, 1H, *H*$_{pyrrole}$), 5.69 (d, $^3J_{HH}$ = 2.8 Hz, 1H, *H*$_{pyrrole}$), 5.66 (d, $^3J_{HH}$ = 2.8 Hz, 1H, *H*$_{pyrrole}$), 5.44 (s, 1H, *H*$_{aldehyde}$), 2.14 (s, 3H, *H*$_{AldehydeCH3}$), 1.84 (s, 3H, *H*$_{CH3}$), 1.66 (s, 3H, *H*$_{CH3}$), 1.64 (s, 3H, *H*$_{CH3}$), 1.63 (s, 3H, *H*$_{CH3}$), 1.59 (s, 3H, *H*$_{CH3}$), 1.54 (s, 3H, *H*$_{CH3}$), 1.37 (s, 3H, *H*$_{CH3}$),

0.86 (s, 3H, H_{CH3}). $^{13}C\{^1H\}$ NMR (DCM-d_2, 150 MHz, 295 K) δ[ppm]: 186.6 (C_q *C4*, identified by $^1H/^{13}C\{^1H\}$ HMBC NMR), 161.6 (CH, *C2*), 150.6 (C_q, $C_{pyrrole}$), 148.7 (C_q, $C_{pyrrole}$), 147.6 (C_q, $C_{pyrrole}$), 147.5 (C_q, $C_{pyrrole}$), 146.9 (C_q, $C_{pyrrole}$), 145.5 (C_q, *C6*), 141.8 (C_q, $C_{pyrrole}$), 136.2 (d, $^4J_{CP}$ = 3.1 Hz, CH, PPh_4^+), 135.1 (C_q, *C9*), 134.8 (d, $^2J_{CP}$ = 10.3 Hz, CH, PPh_4^+), 131.0 (d, $^3J_{CP}$ = 12.9 Hz, CH, PPh_4^+), 128.2 (CH, *C7*), 126.1 (CH, *C3*), 124.1 (CH, *C8*), 117.9 (d, $^1J_{CP}$ = 89.8 Hz, C_q, PPh_4^+), 103.0 (CH, $C_{pyrrole}$), 101.8 (CH, $C_{pyrrole}$), 101.1 (CH, $C_{pyrrole}$), 100.9 (CH, $C_{pyrrole}$), 100.5 (CH, $C_{pyrrole}$), 98.9 (CH, $C_{pyrrole}$), 96.9 (C_q, *C1*), 78.1 (CH, *C5*), 42.9 (C_q), 41.2 (C_q), 38.7 (C_q), 36.6 (C_q), 36.6 (C_{CH3}), 36.1 (C_{CH3}), 36.0 (C_{CH3}), 29.4 (C_{CH3}), 28.4 (C_{CH3}), 27.2 (C_{CH3}), 26.7 (C_{CH3}), 24.2 (C_{CH3}), 21.0 ($C_{PhenylCH3}$). ^{31}P NMR (DCM-d_2, 243 MHz, 295 K) δ[ppm]: 23.23.

Synthesis of [PPh_4][**1***/**1**-*p*-dimethylaminobenzaldehyde]:

To a solution of [PPh_4][**1**] (100 mg, 122 µmol, 1.00 eq.) in 3 ml dichloromethane *p*-dimethylaminobenzaldehyde (18.2 mg, 122 µmol, 1.00 eq.) was added and stirred for 5 min. Full conversion was monitored *via* ^1H NMR spectroscopy. 4 ml *n*-pentane were added to the solution and the brownish solid was separated by filtration from the solution and dried *in vacuo*. [PPh_4][**1***/**1**-*p*-dimethylaminobenzaldehyde] was isolated as a light brownish solid. Suitable crystals for SCXRD were obtained from dichloromethane at -40 °C. ^1H NMR spectroscopy revealed a highly dynamic mixture, which will be discussed in detail in section 5.

Synthesis of [**1***-*p*-dimethylaminobenzaldehyde][$Li(thf)_4$]:

To a solution of [$Li(thf)_4$][**1**-thf] (100 mg, 122 µmol, 1.00 eq.) in 3 ml dichloromethane *p*-dimethylaminobenzaldehyde (18.2 mg, 122 µmol, 1.00 eq.) was added and stirred for 5 min. 4 ml *n*-pentane was added to the solution and the yellow solid was separated by filtration from the solution. The solid was dried after reduced pressure to obtain [$Li(thf)_4$][**1***-*p*-dimethylaminobenzaldehyde] as light yellow solid. ^1H NMR (DCM-d_2, 600 MHz, 295 K) δ[ppm]: 7.07 (d, $^3J_{HH}$ = 5.2 Hz, 1H, *H2*), 6.33 (d, $^3J_{HH}$ = 8.5 Hz, 2H, *H7*), 6.32 (d, $^3J_{HH}$ = 5.2 Hz, 1H, *H3*), 6.27 (d, $^3J_{HH}$ = 8.5 Hz, 1H, *H3*), 6.26 (d, $^3J_{HH}$ = 2.9 Hz, 1H, $H_{pyrrole}$), 6.03 (d, $^3J_{HH}$ = 2.9 Hz, 1H, $H_{pyrrole}$), 6.01 (d, $^3J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 5.90 (d, $^3J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 5.83 (d, $^3J_{HH}$ = 2.8 Hz, 1H, $H_{pyrrole}$), 5.80 (d, $^3J_{HH}$ = 2.8 Hz, 1H, $H_{pyrrole}$), 5.17 (s, 1H, $H_{aldehyde}$), 3.57 (m, 16H, H_{thf}), 2.79 (s, 6H, $H_{AldehydeCH3}$), 1.84 (s, 3H, H_{CH3}), 1.77 (m, 16H, H_{thf}), 1.76 (s, 3H, H_{CH3}), 1.71 (s, 3H, H_{CH3}), 1.70 (s, 3H, H_{CH3}), 1.65 (s, 3H, H_{CH3}), 1.47 (s, 3H, H_{CH3}), 1.43 (s, 3H, H_{CH3}), 0.91 (s, 3H, H_{CH3}). $^{13}C\{^1H\}$ NMR (DCM-d_2, 150 MHz, 295 K) δ[ppm]: 190.1 (C_q *C4*, identified by $^1H/^{13}C\{^1H\}$ HMBC NMR), 160.4 (CH, *C2*), 153.0 (C_q, $C_{pyrrole}$), 150.4 (C_q, $C_{pyrrole}$), 149.9 (C_q, $C_{pyrrole}$), 147.5 (C_q, $C_{pyrrole}$), 147.3 (C_q, $C_{pyrrole}$), 147.1 (C_q, $C_{pyrrole}$), 141.1 (C_q, $C_{pyrrole}$), 131.4 (C_q, $C_{pyrrole}$), 126.7 (CH, *C7*), 111.9 (CH, *C8*), 104.4 (CH, *C3*), 104.3 (CH, $C_{pyrrole}$), 103.2 (CH, $C_{pyrrole}$), 101.8 (CH, $C_{pyrrole}$), 100.8 (CH, $C_{pyrrole}$), 100.1 (CH, $C_{pyrrole}$), 95.6 (C_q, *C1*), 77.5 (CH, *C5*), 68.2 (CH_2, C_{thf}), 42.6 (C_q), 40.7 (C_{NCH3}), 39.1 (C_q), 38.9 (C_{CH3}), 36.5 (C_q), 36.5 (C_{CH3}), 36.4 (C_{CH3}), 36.2 (C_{CH3}), 28.1 (C_{CH3}), 27.1 (C_{CH3}), 26.4 (C_{CH3}), 26.1 (C_{CH3}), 25.9 (C_{thf}), 23.9 (C_{CH3}). ^7Li NMR (DCM-d_2, 233 MHz, 295 K) δ[ppm]: -4.1.

Synthesis of [$Li(thf)_4$][**1***-acetone]:

To a solution of [$Li(thf)_4$][**1**-thf] (100 mg, 122 µmol, 1.00 eq.) in 3 ml tetrahydrofurane, acetone (11.0 µl, 8.7 mg, 151 µmol, 1.20 eq.) was added and stirred for 5 min. Full conversion was detected by ^1H NMR spectroscopy. All volatiles were removed under reduced pressure. [$Li(thf)_4$][**1***-acetone] was obtained as light yellow solid. Suitable crystals for SCXRD were obtained from dichloromethane, dimethoxyethane and *n*-pentane solution at -40 °C. ^1H NMR (DCM-d_2, 600 MHz, 295 K) δ[ppm]: 7.51 (d, $^3J_{HH}$ = 5.0 Hz, 1H, *H2*), 6.84 (d, $^3J_{HH}$ = 5.0 Hz, 1H, *H3*), 6.19 (d, $^3J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 6.01 (d, $^3J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 5.93 (d, $^3J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 5.81 (d, $^3J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 5.79 (m, 2H, $H_{pyrrole}$), 3.58 (m, 16H, H_{THF1}), 1.81 (s, 3H, H_{CH3}), 1.79 (s, 3H, H_{CH3}), 1.77 (m, 16H, H_{THF1}), 1.76 (s, 3H, H_{CH3}), 1.69 (s, 3H, H_{CH3}), 1.60 (s, 3H, H_{CH3}), 1.44 (s, 3H, H_{CH3}), 1.42 (s, 3H, $H_{acetoneCH3}$), 1.40 (s, 3H, H_{CH3}), 0.91 (s, 3H, H_{CH3}), 0.38 (s, 3H, $H_{acetoneCH3}$). $^{13}C\{^1H\}$ NMR (DCM-d_2, 150 MHz, 295 K) δ[ppm]: 187.8 (*C4*), 159.7 (*C2*), 153.1 ($C_{q,pyrrole}$), 150.4 ($C_{q,pyrrole}$), 148.3 ($C_{q,pyrrole}$), 147.3 ($C_{q,pyrrole}$), 146.5 ($C_{q,pyrrole}$), 141.2 ($C_{q,pyrrole}$), 129.0 (*C3*), 103.5 ($C_{CH,pyrrole}$), 103.4 ($C_{CH,pyrrole}$), 103.0 ($C_{CH,pyrrole}$), 100.7 ($C_{CH,pyrrole}$), 100.7 ($C_{CH,pyrrole}$), 100.3 ($C_{CH,pyrrole}$), 96.6 (*C1*), 77.6 (*C5*), 68.2 (C_{THF}), 42.2 (C_q), 38.8 (C_q), 38.4 (C_{CH3}), 36.5 (C_q), 36.5 (C_{CH3}), 36.4 (C_q), 35.6 (C_{CH3}), 30.0

($C_{acetoneCH3}$), 29.9 (C_{CH3}), 29.0 ($C_{acetoneCH3}$), 27.7 (C_{CH3}), 27.1 (C_{CH3}), 26.1 (C_{CH3}), 25.8 (C_{THF}), 24.9 (C_{CH3}). ^{7}Li NMR (DCM-d_2, 233 MHz, 295 K) δ[ppm]: -4.6.

Synthesis of [PPh_4][**1**-acetone]:

To a solution of [PPh_4][**1**] (100 mg, 122 µmol, 1.00 eq.) in 3 ml dichloromethane acetone (11.0 µl, 8.7 mg, 151 µmol, 1.20 eq.) was added and stirred for 5 min. Full conversion was detected by ^{1}H NMR spectroscopy. All volatiles were removed under reduced pressure. [**1**-acetone][PPh_4] was obtained as yellow solid. Due to strong line broadening no appropriate $^{13}C\{^{1}H\}$ NMR spectra was obtained. For further discussion of the dynamic behavior, see section 4. ^{1}H NMR (DCM-d_2, 600 MHz, 295 K) δ[ppm]: 7.855 (m, 4H, PPh_4^+), 7.68 (m, 8H, PPh_4^+), 7.57 (m, 8H, PPh_4^+), 5.76 (s, 8H, $H_{pyrrole}$), 1.62 (s, 12H, H_{CH3}), 1.62 (s, 3H, $H_{acetoneCH3}$), 1.41 (s, 12H, H_{CH3}), 1.26 (s, 3H, $H_{acetoneCH3}$). ^{31}P NMRP NMR (DCM-d_2, 243 MHz, 295 K) δ[ppm]: 23.20.

Synthesis of [$Li(thf)_4$][**1***-cyclopentanone]:

To a solution of [$Li(thf)_4$][**1**-thf] (100 mg, 122 µmol, 1.00 eq.) in 3 ml tetrahydrofurane, cyclopentanone (12.7 mg, 151 µmol, 1.20 eq.) was added and stirred for 5 min. Full conversion was monitored by ^{1}H NMR spectroscopy. 4 ml *n*-pentane were added to the solution and the yellow solid was separated by filtration from the solution. [$Li(thf)_4$][**1***-cyclopentanone] was obtained as yellow solid. ^{1}H NMR (DCM-d_2, 600 MHz, 295 K) δ[ppm]: 7.55 (d, $^{3}J_{HH}$ = 5.0 Hz, 1H, *H2*), 6.85 (d, $^{3}J_{HH}$ = 5.0 Hz, 1H, *H3*), 6.18 (d, $^{3}J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 6.00 (d, $^{3}J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 5.93 (d, $^{3}J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 5.81 (d, $^{3}J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 5.80 (d, $^{3}J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 5.79 (d, $^{3}J_{HH}$ = 3.1 Hz, 1H, $H_{pyrrole}$), 3.58 (m, 16H, H_{THF1}), 1.86 (m, 1H, H_{CH2}), 1.80 (s, 3H, H_{CH3}), 1.77 (m, 16H, H_{THF1}), 1.77 (s, 3H, H_{CH3}), 1.75 (s, 3H, H_{CH3}), 1.68 (s, 3H, H_{CH3}), 1.60 (s, 3H, H_{CH3}), 1.56 (m, 3H, H_{CH2}), 1.44 (s, 3H, H_{CH3}), 1.42 (s, 3H, H_{CH3}), 1.40 (s, 1H, H_{CH2}), 1.21 (m, 1H, H_{CH2}), 0.91 (s, 3H, H_{CH3}), 0.91 (s, 1H, H_{CH2}), 0.76 (s, 1H, H_{CH2}). $^{13}C\{^{1}H\}$ NMR (DCM-d_2, 150 MHz, 295 K) δ[ppm]: 186.8 (*C4*), 159.9 (*C2*), 153.1 ($C_{q,pyrrole}$), 150.3 ($C_{q,pyrrole}$), 148.7 ($C_{q,pyrrole}$), 147.3 ($C_{q,pyrrole}$), 146.7 ($C_{q,pyrrole}$), 141.4 ($C_{q,pyrrole}$), 128.6 (*C3*), 103.4 ($C_{CH,pyrrole}$), 103.1 ($C_{CH,pyrrole}$), 103.0 ($C_{CH,pyrrole}$), 100.8 ($C_{CH,pyrrole}$), 100.7 ($C_{CH,pyrrole}$), 100.3 ($C_{CH,pyrrole}$), 96.3 (*C1*), 88.4 (*C5*), 68.2 (C_{THF}), 42.2 (C_q), 39.3 (C_{CH2}), 38.8 (C_q), 38.5 (C_{CH3}), 37.6 (C_{CH2}), 36.5 (C_{CH3}), 36.4 (C_q), 36.3 (C_q), 36.2 (C_{CH3}), 29.1 (C_{CH3}), 27.5 (C_{CH3}), 27.1 (C_{CH3}), 26.2 (C_{CH3}), 25.8 (C_{THF}), 24.1 (C_{CH3}), 23.5 (C_{CH2}), 21.0 (C_{CH2}). ^{7}Li NMR (DCM-d_2, 243 MHz, 295 K) δ[ppm]: -4.7.

Synthesis of [PPh_4][**1**-cyclopentanone]:

To a solution of [PPh_4][**1**] (100 mg, 122 µmol, 1.00 eq.) in 3 ml dichloromethane, cyclopentanone (12.7 mg, 151 µmol, 1.20 eq.) was added and stirred for 5 min. Full conversion was monitored by ^{1}H NMR spectroscopy. [PPh_4][**1**-cyclopentanone] was obtained as light yellow solid.

^{1}H NMR (DCM-d_2, 600 MHz, 295 K) δ[ppm]: 7.83-7.80 (m, 4H, PPh_4^+), 7.67-7.65 (m, 8H, PPh_4^+), 7.56-7.52 (m, 8H, PPh_4^+), 5.78 (s, 4H, $H_{pyrrole}$), 5.74 (s, 4H, $H_{pyrrole}$), 1.61 (s, 6H, H_{CH3}), 1.59 (s, 6H, H_{CH3}), 1.52 (s, 4H, H_{CH2}), 1.42 (s, 4H, H_{CH2}), 1.39 (s, 3H, H_{CH3}), 1.24 (s, 3H, H_{CH3}). $^{13}C\{^{1}H\}$ NMR (DCM-d_2, 150 MHz, 295 K) δ[ppm]: 148.0 ($C_{q,pyrrole}$), 147.1 ($C_{q,pyrrole}$), 136.2 (d, $^{4}J_{CP}$ = 3.1 Hz, CH, PPh_4^+), 134.8 (d, $^{2}J_{CP}$ = 10.3 Hz, CH, PPh_4^+), 131.0 (d, $^{3}J_{CP}$ = 12.9 Hz, CH, PPh_4^+), 117.9 (d, $^{1}J_{CP}$ = 89.8 Hz, C_q, PPh_4^+), 101.8 ($C_{CH,pyrrole}$), 99.7 ($C_{CH,pyrrole}$), 41.3 (C_{CH3}), 39.8 (C_{CH2}), 37.4 (C_{CH3}), 36.0 (C_q), 35.8 (C_q), 34.2 (C_{CH3}), 26.0 (C_{CH3}), 23.3 (C_{CH2}).^{31}P NMR (DCM-d_2, 243 MHz, 295 K) δ[ppm]: 23.2.

Synthesis of [PPh_4][**1**-formamide]:

To a solution of [PPh_4][**1**] (100 mg, 122 µmol, 1.00 eq.) in 3 ml dichloromethane, formamide (5.5 mg, 122 µmol, 1.00 eq.) was added and stirred for 5 min. Full conversion was monitored by ^{1}H NMR spectroscopy. Crystallization started immediately at rt and produced suitable material for SCXRD measurements. ^{1}H NMR (DCM-d_2, 200 MHz, 295 K) δ[ppm]: 7.86-7.84 (m, 4H, PPh_4^+), 7.69-7.66 (m, 8H, PPh_4^+), 7.54-7.53 (m, 8H, PPh_4^+), 5.77 (s, 8H, $H_{pyrrole}$), 1.58 (s, 12H, H_{CH3}), 1.33 (s, 12H, H_{CH3}). $^{13}C\{^{1}H\}$ NMR (DCM-d_2, 150 MHz, 295 K) δ[ppm]: 163.9 ($C_{Aldehyde}$) 147.6 ($C_{q,pyrrole}$), 136.1 (d, $^{4}J_{CP}$ = 3.1 Hz, CH, PPh_4^+), 134.8

(d, $^{2}J_{CP}$ = 10.3 Hz, CH, *PPh*$_4^+$), 131.0 (d, $^{3}J_{CP}$ = 12.9 Hz, CH, *PPh*$_4^+$), 117.9 (d, $^{1}J_{CP}$ = 89.8 Hz, C_q, *PPh*$_4^+$), 101.1 ($C_{CH,pyrrole}$), 36.0 (C_{CH3}). ^{31}P NMR (DCM-d_2, 243 MHz, 295 K) δ[ppm]: 23.2.

Synthesis of [PPh_4][**1**-dimethylformamide]:

To a solution of [PPh_4][**1**] (100 mg, 122 µmol, 1.00 eq.) in 3 ml dichloromethane, dimethylformamide (8.9 mg, 122 µmol, 1.00 eq.) was added and stirred for 5 min. All volatiles were removed under reduced pressure. [PPh_4][**1**-dimethylformamide] was obtained as light yellow solid. Suitable crystals for SCXRD were obtained from a dichloromethane solution at rt. Due to strong line broadening no appropriate $^{13}C\{^{1}H\}$ NMR could be obtained. ^{1}H NMR (DCM-d_2, 600 MHz, 295 K) δ[ppm]: 7.83 (m, 4H, *PPh*$_4^+$), 7.67 (m, 8H, *PPh*$_4^+$), 7.56-7.52 (m, 8H, *PPh*$_4^+$), 5.75 (s, 8H, $H_{pyrrole}$), 5.03 (s, 1H, $H_{CH,dimethylformamide}$), 2.71 (s, 3H, $H_{CH3,dimethylformamide}$), 2.64 (s, 3H, $H_{CH3,dimethylformamide}$), 1.60 (s, 12H, H_{CH3}), 1.33 (s, 12H, H_{CH3}). ^{31}P NMR (DCM-d_2, 243 MHz, 295 K) δ[ppm]: 23.2.

3. $^{13}CO_2$ labeling experiments

[Li(thf)$_4$][**1**-thf] was dissolved in THF-d_8, the solution degassed by 3 freeze-pump-thaw cycles and 1 bar $^{13}CO_2$ was added. After completion of the reaction, monitored by ^{1}H and ^{13}C{^{1}H} NMR spectroscopy, the solution was degassed 3 times and 1 bar $^{12}CO_2$ was added. The exchange was studied at room temperature over 24 h. Characteristic regions are shown in figures S 1 and S 2.

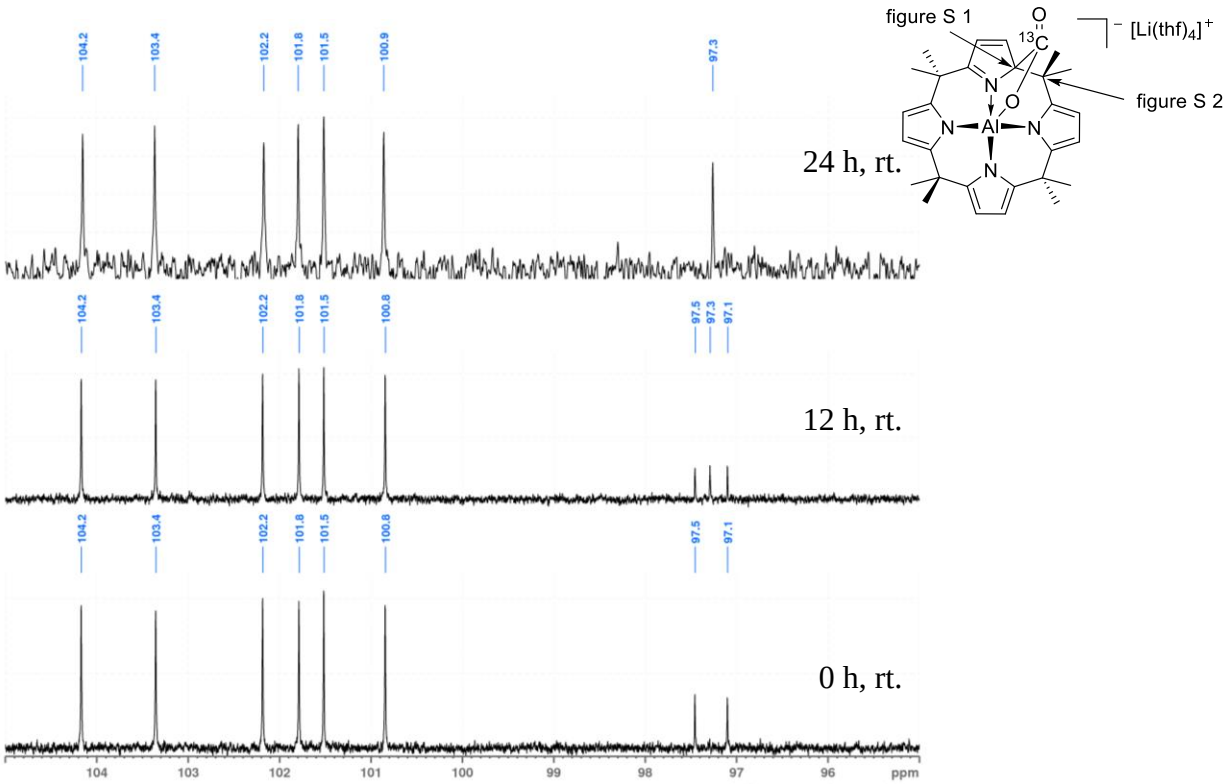


Figure S 1: Stacked ^{13}C{^{1}H} NMR (150 MHz, THF-d_8, 295 K) spectra showing an exchange of isotope-labeled $^{13}CO_2$ against non-labeled $^{12}CO_2$ at room temperature. It is monitored by the doublet (δ[ppm]: 97.5 and 97.1, $J_{13C,12C}$ = 53.5 Hz) at 0 h at room temperature of [Li(thf)$_4$][**1***-$^{13}CO_2$], considered carbon atom can be found in the sketch above, in between after 12 h at room temperature the singlet (δ[ppm]: 97.3) of the [Li(thf)$_4$][**1***-CO_2] is arising, showing full conversion after 24h at room temperature.

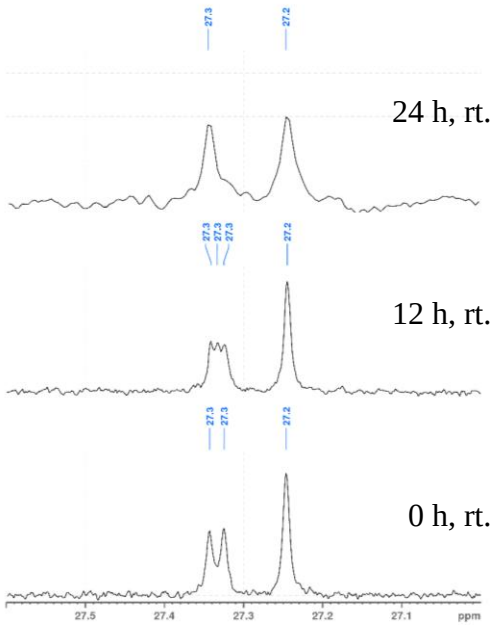


Figure S 2: Stacked $^{13}C\{^{1}H\}$ NMR (150 MHz, THF-d_8, 295 K) spectra showing an exchange of isotope-labeled $^{13}CO_2$ against non-labeled $^{12}CO_2$ at room temperature. It is monitored by the doublet (δ[ppm]: 27.3 $J_{13C,12C}$ = 2.8 Hz) at 0 h at room temperature of [Li(thf)$_4$][**1***-$^{13}CO_2$], considered carbon atom can be found in the sketch above, in between after 12 h at room temperature the singlet of the [Li(thf)$_4$][**1***-CO_2] is arising, showing full conversion after 24h at room temperature.

4. Variable temperature ^{1}H NMR measurements of [PPh$_4$][1-acetone]

Low temperature ^{1}H NMR measurements of a sample of [PPh$_4$][**1**-acetone] in DCM-d_2 revealed a shift in the chemical equilibrium between [PPh$_4$][**1**-acetone] and [PPh$_4$][**1***-acetone] toward the latter at low temperatures. However, the equilibrium is still lying clearly on the side of [PPh$_4$][**1**-acetone].

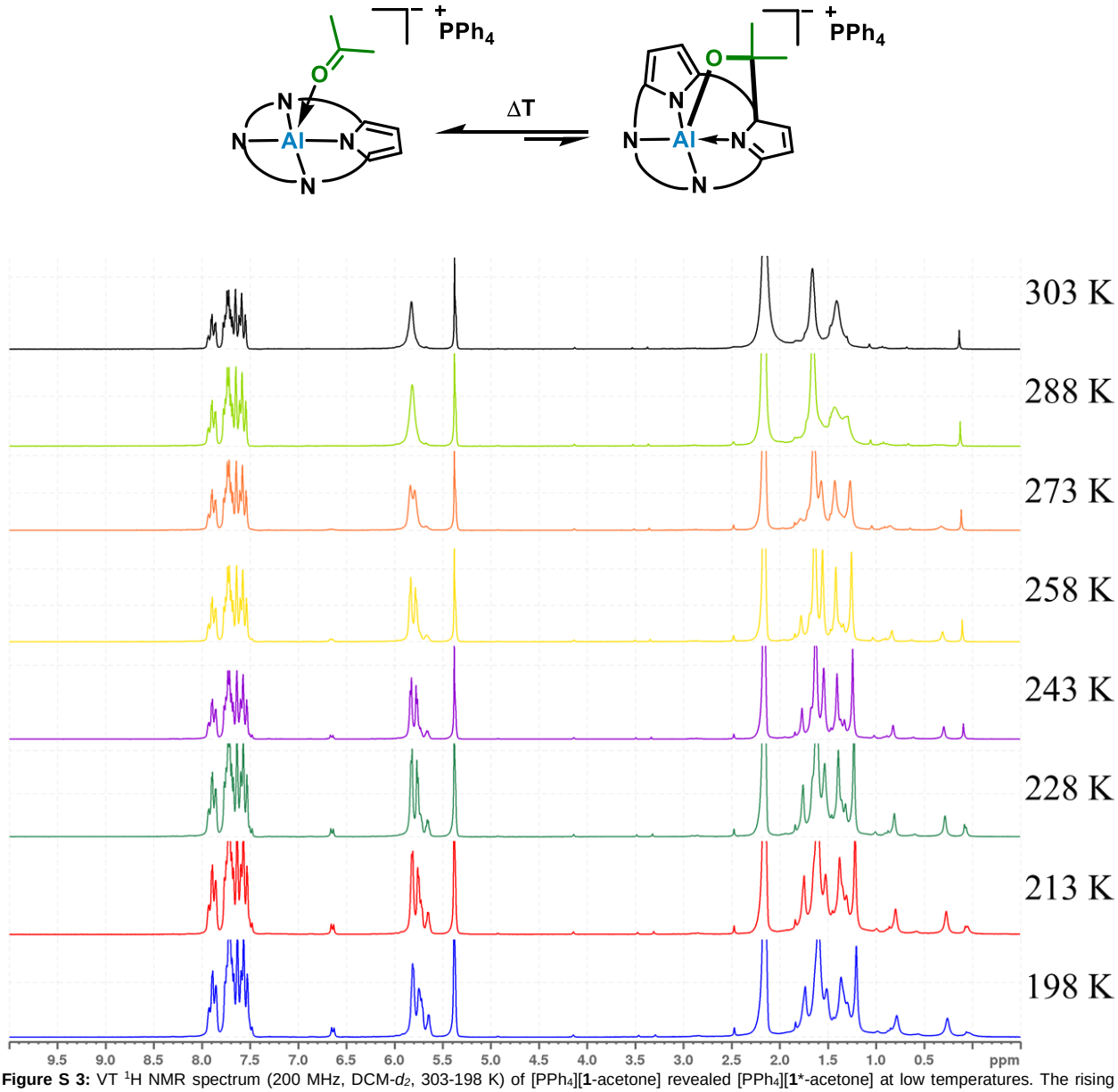


Figure S 3: VT ^{1}H NMR spectrum (200 MHz, DCM-d_2, 303-198 K) of [PPh$_4$][**1**-acetone] revealed [PPh$_4$][**1***-acetone] at low temperatures. The rising doublet at around 6.6 ppm indicates [PPh$_4$][**1***-acetone].

5. Dynamics and different Isomers of [1-*p*DMA-BA][PPh_4]

Mixing *p*-dimethylaminobenzaldehyde 1:1 with [PPh_4][**1**] in dichloromethane-d_2 at room temperature yields a ^{1}H NMR spectrum (see fig. S 4) that shows broad peaks of the substrate and the aluminate anion. Due to the dynamics at room temperature, the sample was cooled to -25 °C and full characterization utilizing multinuclear NMR measurements was conducted. A discrete ^{1}H NMR spectrum (see fig. S 5) was obtained, showing four different species. These were identified by the aromatic signal sets of the *p*-dimethylaminobenzalehyde considering ^{1}H ^{1}H COSY cross peak analysis (see fig. S 7). The corresponding signal sets are marked with green connecting arrows in figure S 5. Manifesting the dynamic exchange of the species, various ^{1}H ^{1}H NOESY- exchange cross peaks (see fig. S 8) are obtained (marked with dashed orange arrows in fig. S 5), none of them within the same signal set. Moreover, the exchange from sigma to 1,2-adducts is highlighted by the methyl signal sets of *p*-dimethylaminobenzalehyde at δ = 2.7 and 3.0 ppm. The four isomers were calculated by DFT calculations and are shown in figure S 6 (for the comparison of the energies of the isomers see section 12.2). Because of the four isomers and the dynamics, no meaningful ^{13}C{^{1}H} NMR spectrum could be obtained.

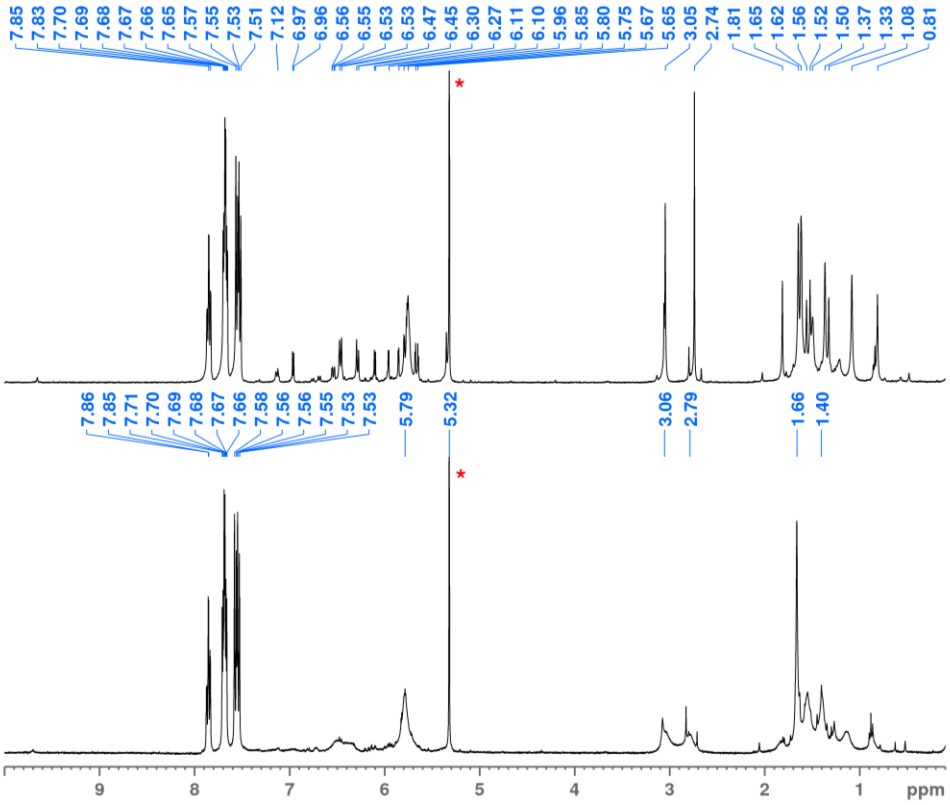


Figure S 4: ^{1}H NMR (400 MHz, DCM-d_2, 295 K / 270 K) spectra of [PPh_4][**1**] with *p*DMA-BA at room temperature (bottom) and 270 K showing four isomers.

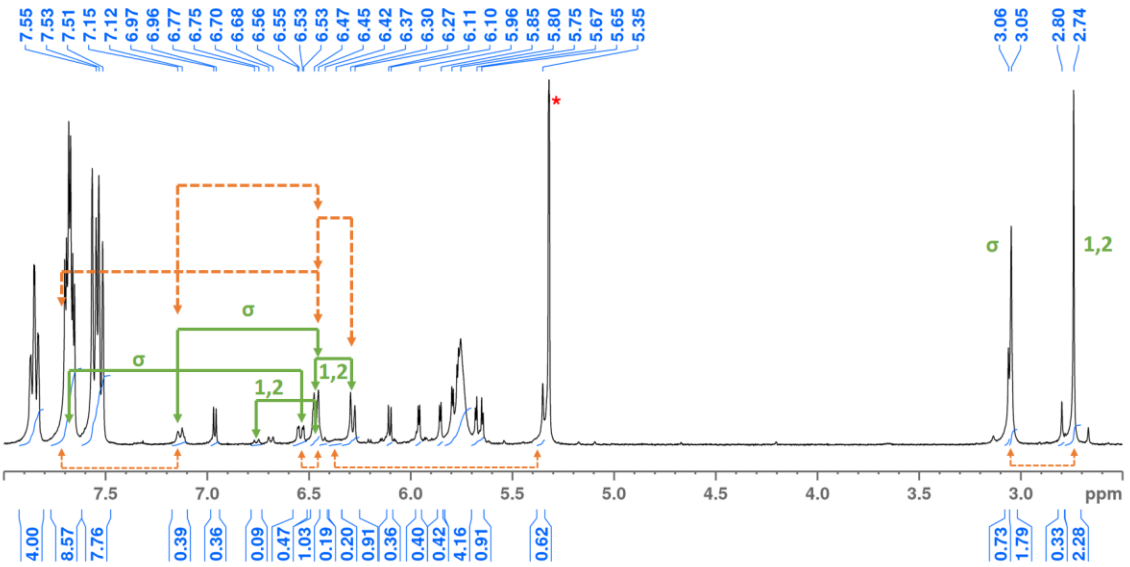


Figure S 5: ^{1}H NMR (400 MHz, DCM-d_2, 270 K) spectrum of [PPh_4][**1**] with *p*DMA-BA at 270 K showing four different isomers (see. fig. S 6). Orange-dashed arrows dynamic exchange pathways found by ^{1}H ^{1}H NOESY NMR, green arrows indicate connections found by ^{1}H^{1}H COSY NMR of different coordination of *p*DMA-BA.

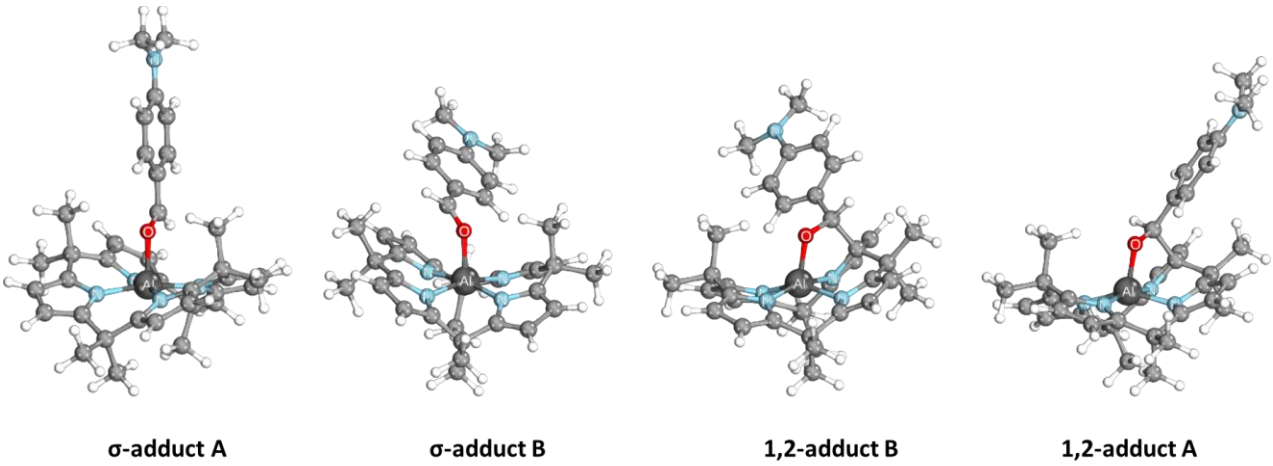


Figure S 6 Visualization of different Isomers of [**1**-*p*DMA-BA]$^{-}$and [**1***-*p*DMA-BA]$^{-}$.

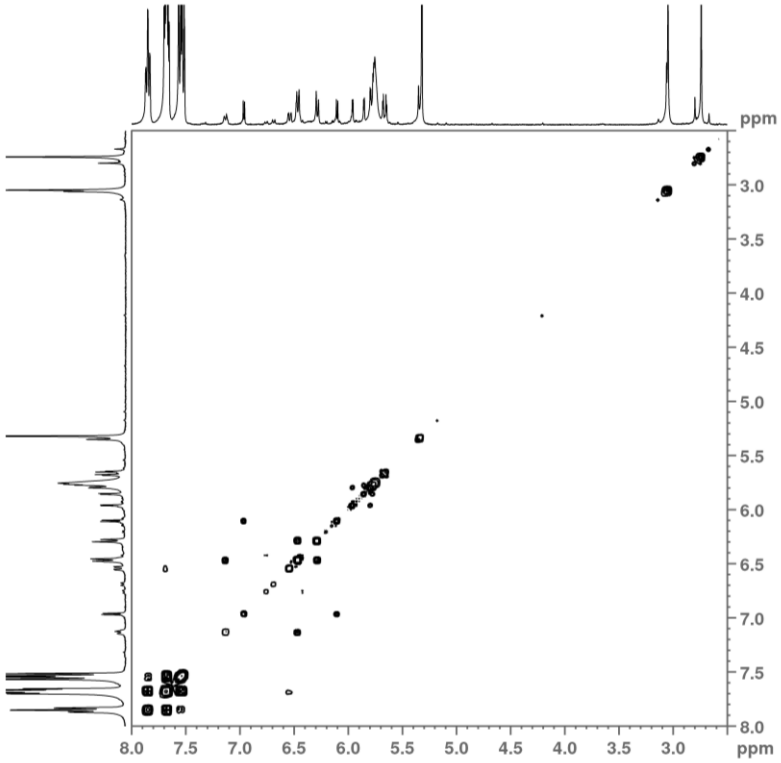


Figure S 7: ^{1}H ^{1}H COSY NMR (400 MHz, DCM-d_2, 270 K) spectrum of a mixture of isomers of [PPh_4][**1**] with *p*DMA-BA.

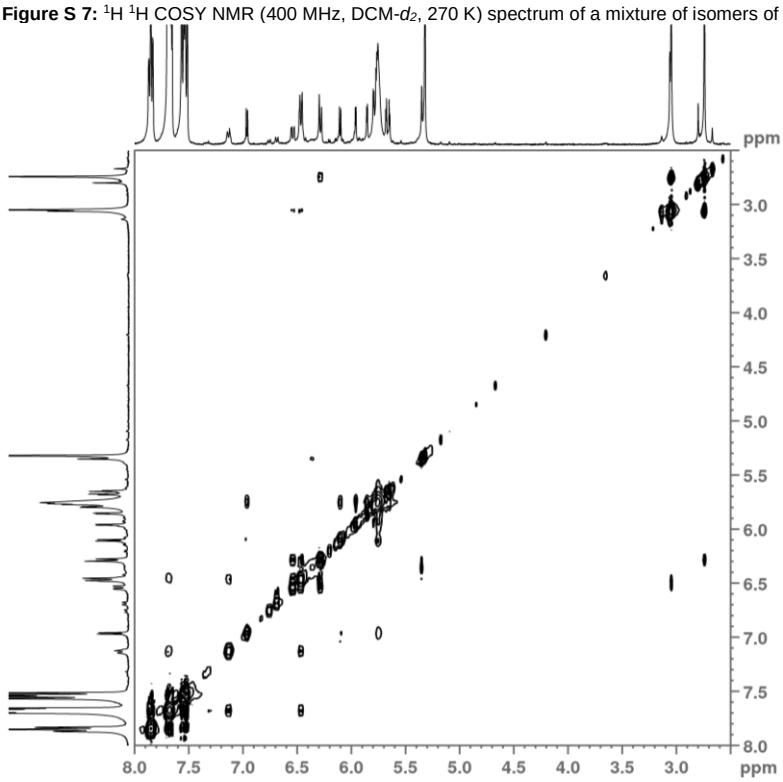
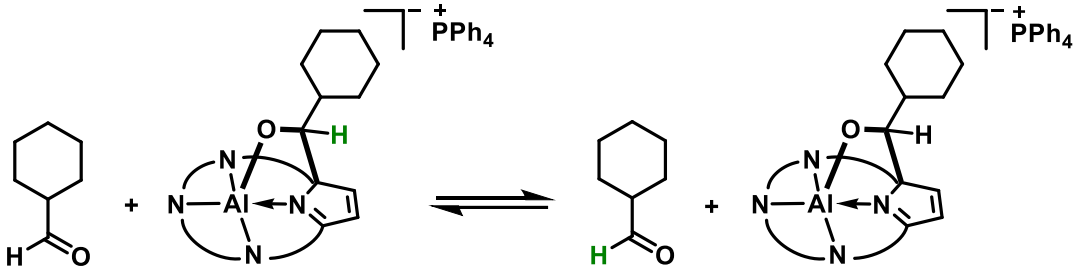


Figure S 8: ^{1}H ^{1}H NOESY NMR (400 MHz, DCM-d_2, 270 K) spectrum of a mixture of isomers of [PPh_4][**1**] with *p*DMA-BA.

6. Exchange of [PPh_4][1*-CyA] monitored by 2D EXSY NMR spectroscopy



The shown reaction was studied via EXSY NMR spectroscopy using cross-peak integration with three different concentrations (22 mM, 34 mM, 64 mM, see fig S 9) of additional cyclohexanecarboxaldehyde at rt in DCM-d_2. The aldehyde-hydrogen atom was fount appropriate for quantitative evaluation in both the free ($\delta = 9.58$, d) and the bound substrate ($\delta = 4.14$, d) as no signal overlapping occurred. Concentration independence is shown in figure S 10 – S 12.

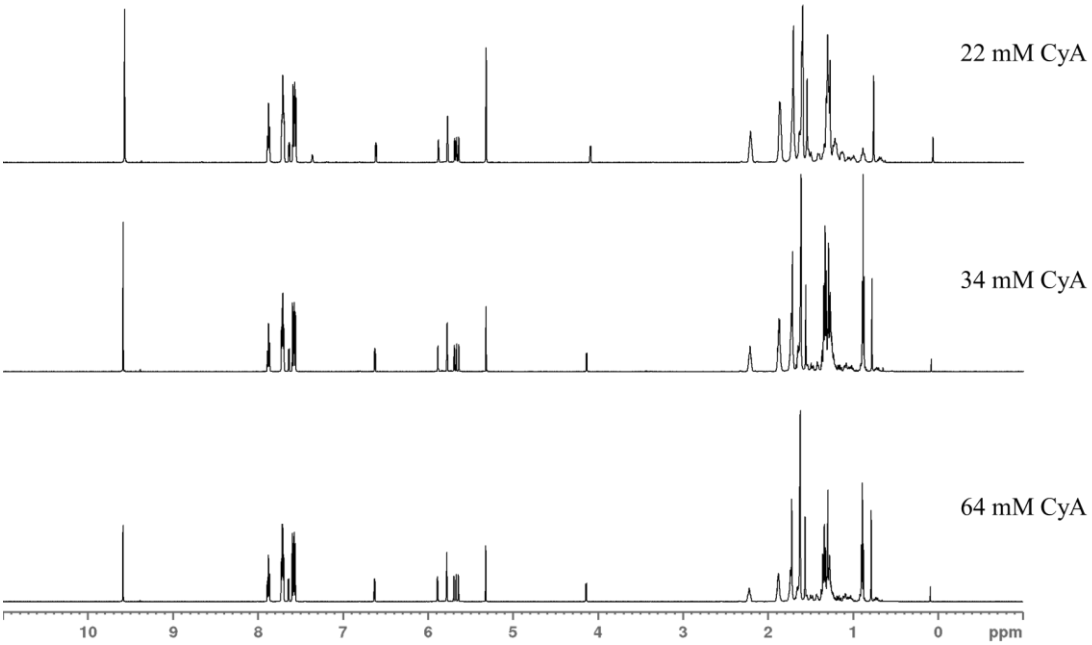


Figure S 9: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) of [PPh_4][**1***-cyclohexanecarboxaldehyde] with three different concentrations of free CyA (22 mM, 34 mM, 64 mM).

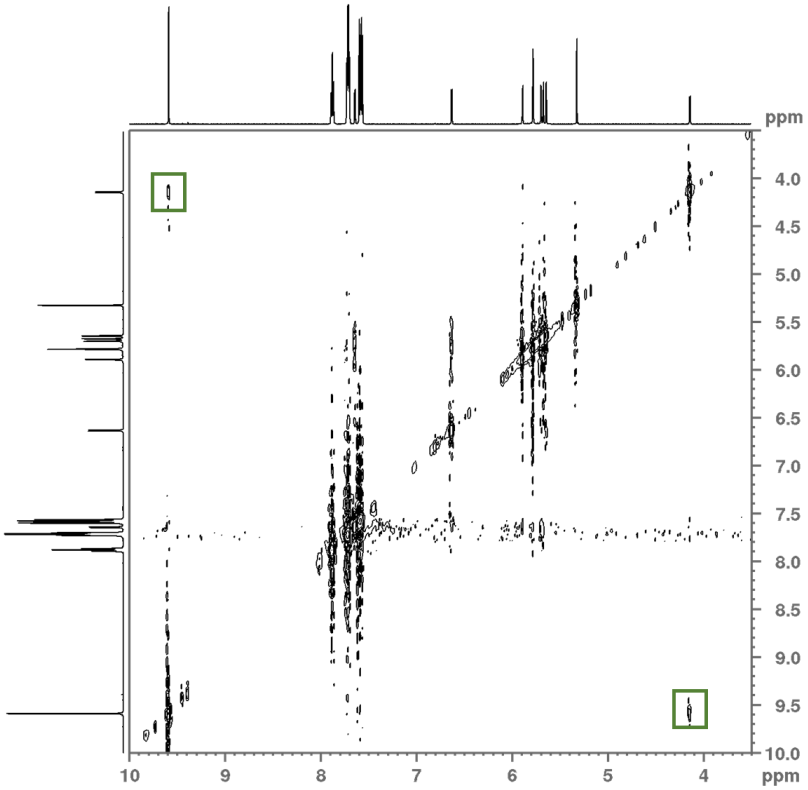


Figure S 10: ^{1}H ^{1}H NOESY NMR (600 MHz, DCM-d_2, 295 K) of [PPh_4][**1***-cyclohexanecarbaoxaldehyde]. Parameters: d1 = 40 s, d8 = 0.4 s, conc. CyA: 22 mMol.

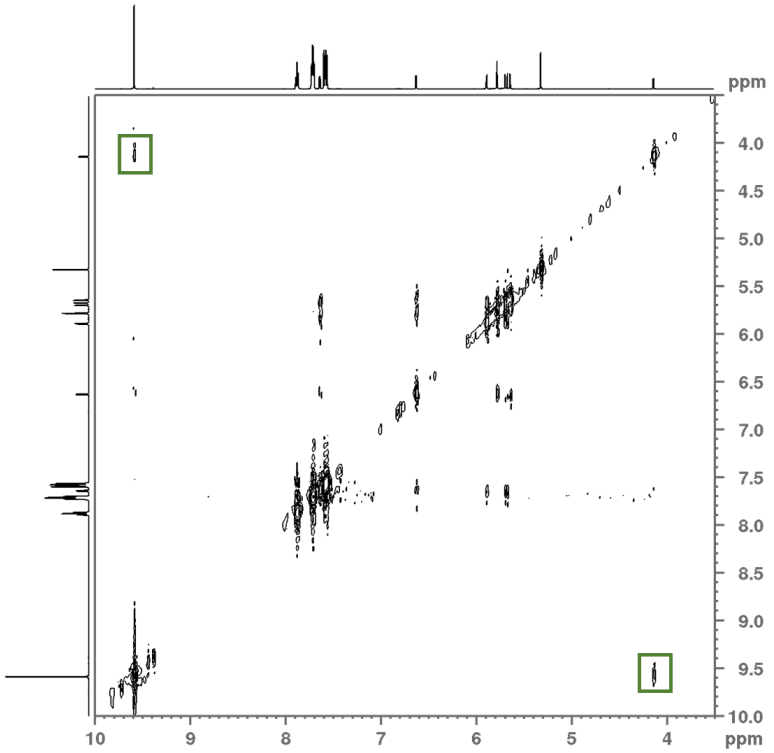


Figure S 11: ^{1}H ^{1}H NOESY NMR (600 MHz, DCM-d_2, 295 K) of [PPh_4][**1***-cyclohexanecarbaoxaldehyde]. Parameters: d1 = 40 s, d8 = 0.4 s, conc. CyA: 34 mMol.

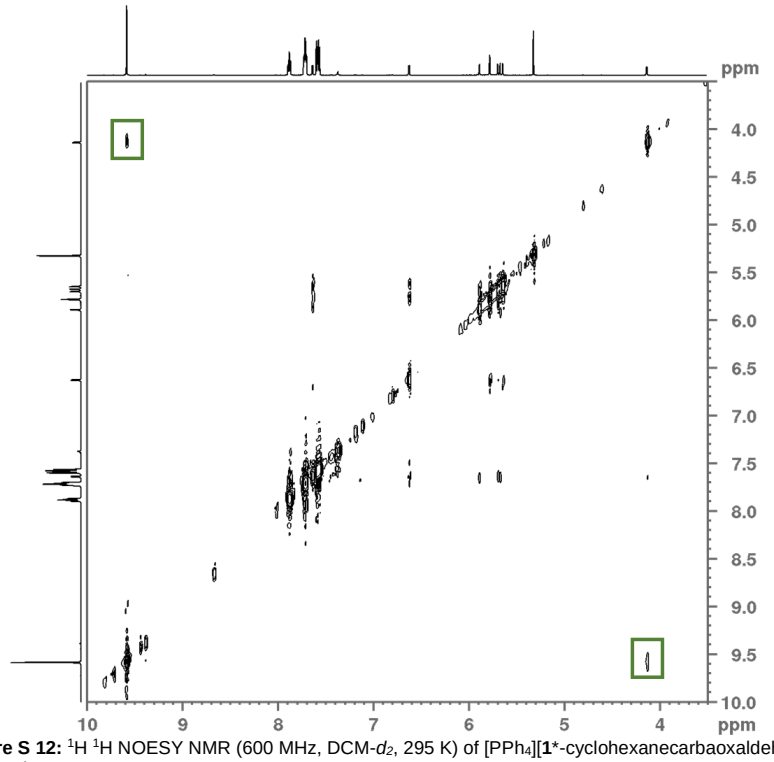


Figure S 12: ^{1}H ^{1}H NOESY NMR (600 MHz, DCM-d_2, 295 K) of [PPh_4][**1***-cyclohexanecarbaoxaldehyde]. Parameters: d1 = 40 s, d8 = 0.4 s, conc. CyA: 64 mMol.

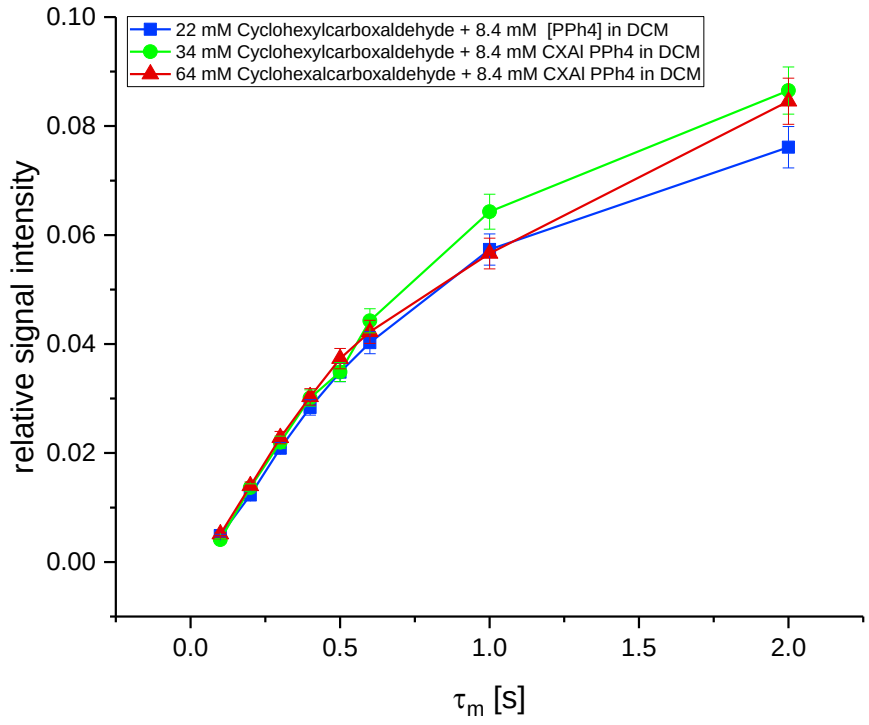


Figure S 13: EXSY plot of relative signal intensities vs. mixing time of the considered integrals marked in figure S 10 – S 12.

Table S 1: Integrals obtained from EXSY spectroscopy over different mixing times, following the exchange from free CyA to bound CyA with [**1**][PPh_4].

	22 mM CyA + 8.4 mM [PPh_4][1] in DCM			34 mM CyA + 8.4 mM [PPh_4][1] in DCM			64 mM CyA + 8.4 mM [PPh_4][1] in DCM		
τ_m	Exchange	free CyA	Bound CyA	Exchange	free CyA	Bound CyA	Exchange	free CyA	Bound CyA
0.1	0.005	1.610	1.000	0.004	2.585	1.000	0.005	4.495	1.000
0.2	0.012	1.586	0.939	0.014	2.499	0.941	0.014	4.497	0.935
0.3	0.021	1.531	0.832	0.022	2.489	0.839	0.023	4.438	0.863
0.4	0.028	1.563	0.760	0.030	2.460	0.758	0.030	4.457	0.745
0.5	0.035	1.524	0.687	0.035	2.421	0.691	0.037	4.416	0.684
0.6	0.040	1.525	0.613	0.044	2.280	0.651	0.042	4.432	0.632
1	0.057	1.454	0.372	0.064	2.301	0.366	0.057	4.287	0.382
2	0.076	1.286	0.147	0.087	1.992	0.134	0.085	3.961	0.146

$K_{forward}$ determined with EXSY Calc for all three concentrations from cross peak exchange:

c(CyA)	$k_{forward}$
22 mM	0.08016667
34 mM	0.08183333
64 mM	0.08316667

Based on this median rate constant $k_{forward}$ = 0.08 s^{-1} and the Eyring-Polanyi equation

$$k = \frac{k_B T}{h} exp\left(-\frac{\Delta G^{\neq}}{RT}\right)$$

the energy barrier of the exchange could be determined to 79.4 kJ/mol.

7. Influence of Li^+ on the addition mode

7.1. Influence on the coordination mode

As discussed in the manuscript, the binding mode of substrates toward the calix[4]pyrrolato-aluminate can be controlled by the influence of the counter cation. The following spectra unfold this feature. In any case, full conversion of σ-adducts to 1,2 adducts proceeded by adding any soluble Li^+ source. Exemplarily, the different coordination of cyclopentanone with [PPh_4][**1**] and [$Li(thf)_4$][**1**] is shown in figure S 14 and S 15. Taking a sample of [PPh_4][**1**-*p*DMA-BA], showing strong dynamics at room temperature (see. section 5) and adding LiI led directly to the 1,2 adduct shown in figure S 16. Moreover, adding LiI to a sample of [PPh_4][**1**-acetone], which presented high exchange between bound and free acetone, detected by ^{1}H ^{1}H NOESY NMR spectroscopy at rt (see fig. S 17), led to [$Li(L)_n$][**1***-acetone], showing just negligible exchange between free and bound acetone, detected by ^{1}H ^{1}H NOESY NMR (see fig. S 18 and S 19). The limits of this concept are defined by formamide as a substrate. The addition of Li^+ to [PPh_4][**1**-formamide] in DCM-d_2 did not induce MLC-type binding and [**1***-formamide] was not obtained (see fig. S 20).

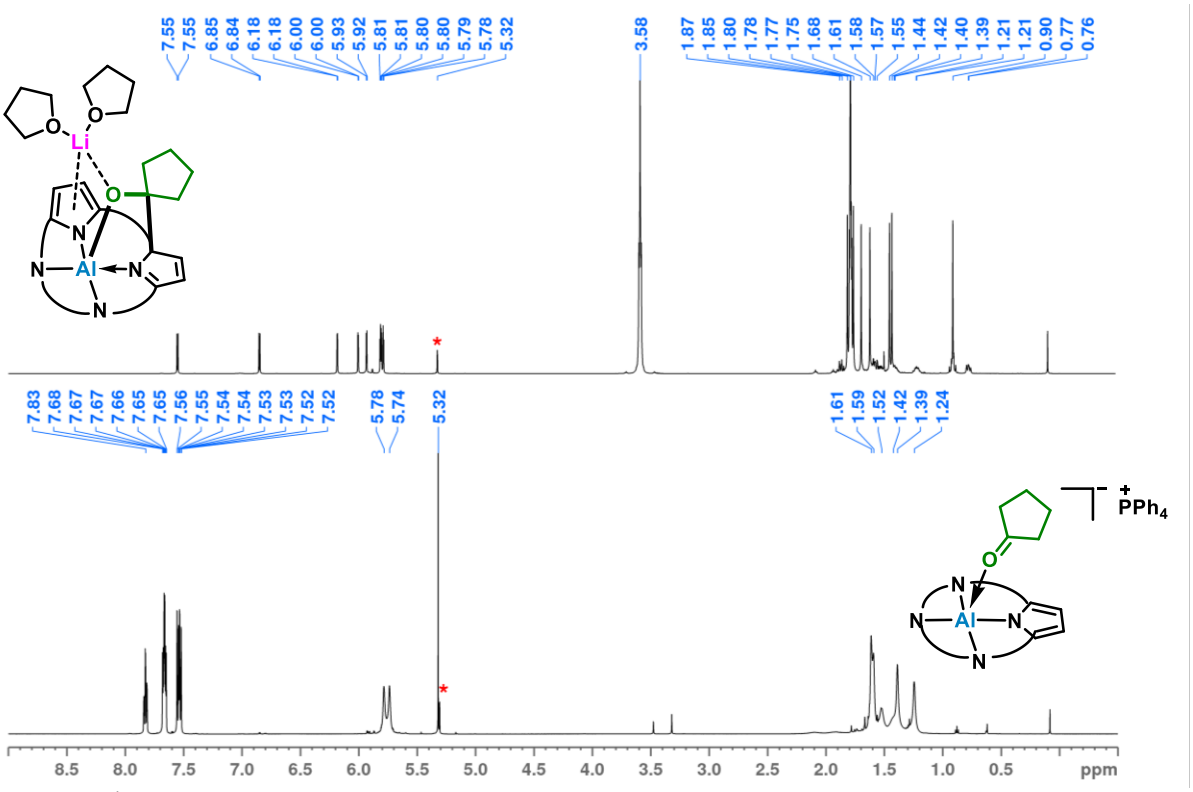


Figure S 14: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectra of σ-coordinated [PPh_4][**1**-cyclopentanone] and 1,2 bound [$Li(thf)_2$][**1***-cyclopentanone], demonstrating the "click" due to coordination of Li^+.

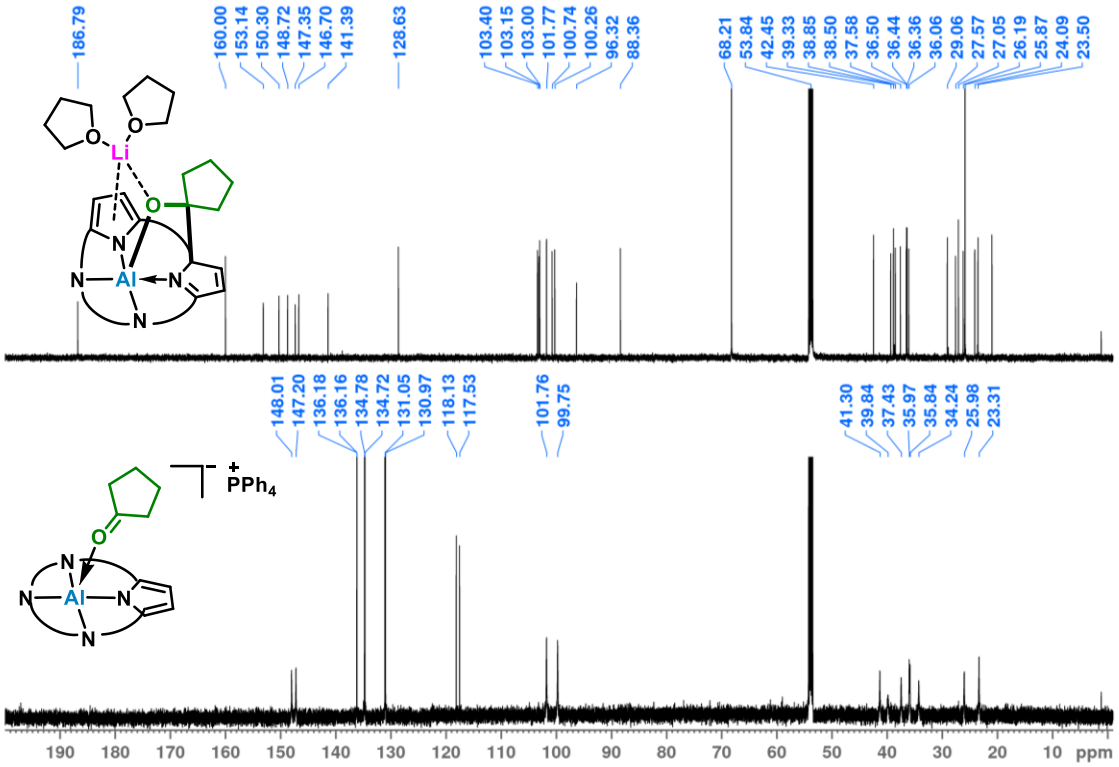


Figure S 15: $^{13}C\{^{1}H\}$ NMR (150 MHz, DCM-d_2, 295 K) spectra of σ-coordinated [PPh_4][**1**-cyclopentanone] and 1,2 bound [Li(thf)$_2$][**1***-cyclopentanone], demonstrating the "click" due to coordination of Li^+.

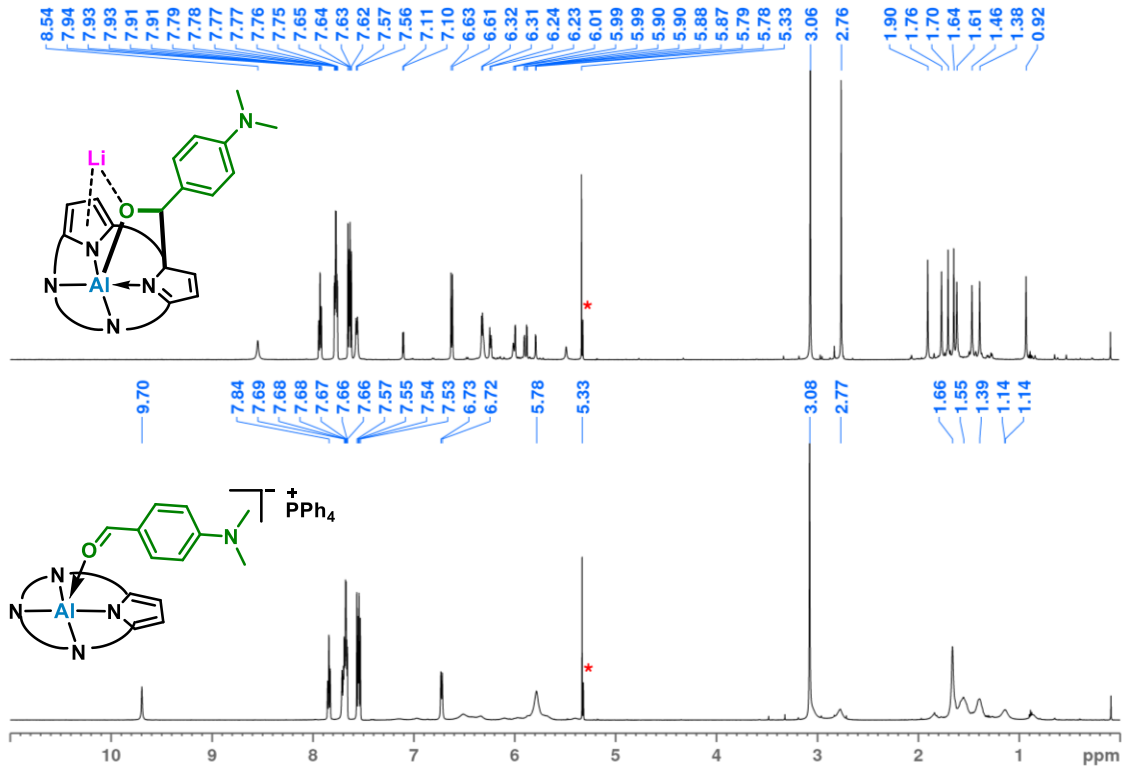


Figure S 16: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectra of σ-coordinated [PPh_4][**1**-*p*DMA-BA] and 1,2 bound [Li][**1***- *p*DMA-BA], demonstrating the "click" due to coordination of Li^+.

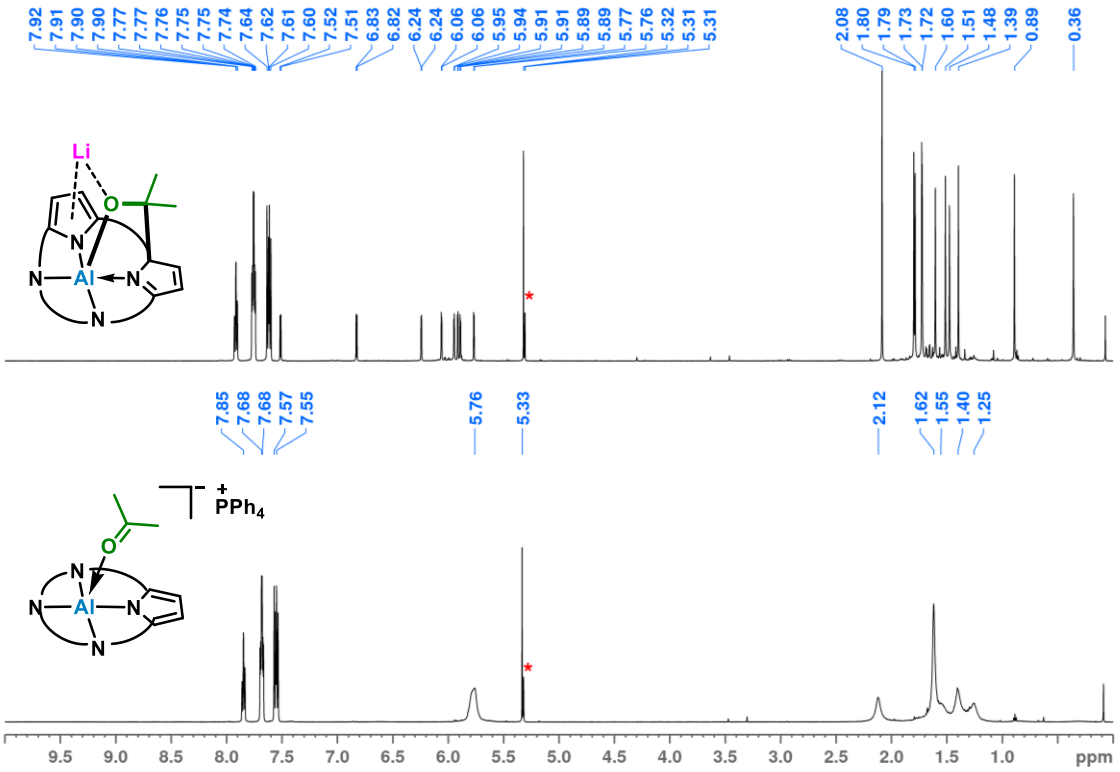


Figure S 17: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectra of σ-coordinated [PPh_4][**1**-acetone] and 1,2 bound [Li][**1***-acetone], demonstrating the "click" due to coordination of Li^+.

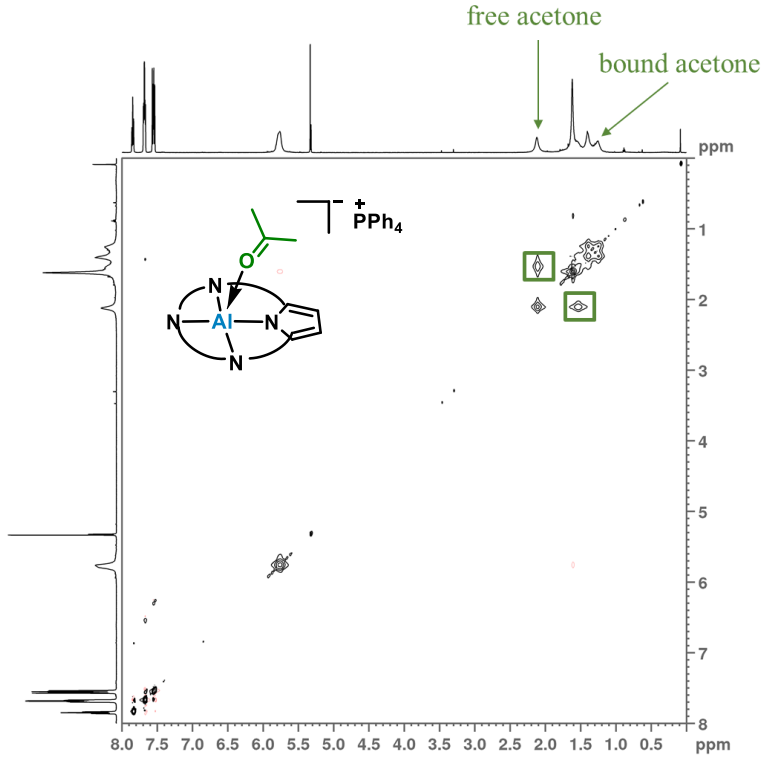


Figure S 18: ^{1}H ^{1}H NOESY NMR (600 MHz, DCM-d_2, 295 K, τ_m = 300 ms) spectra of σ-coordinated [PPh_4][**1**-acetone] exhibiting strong exchange between bound and free acetone.

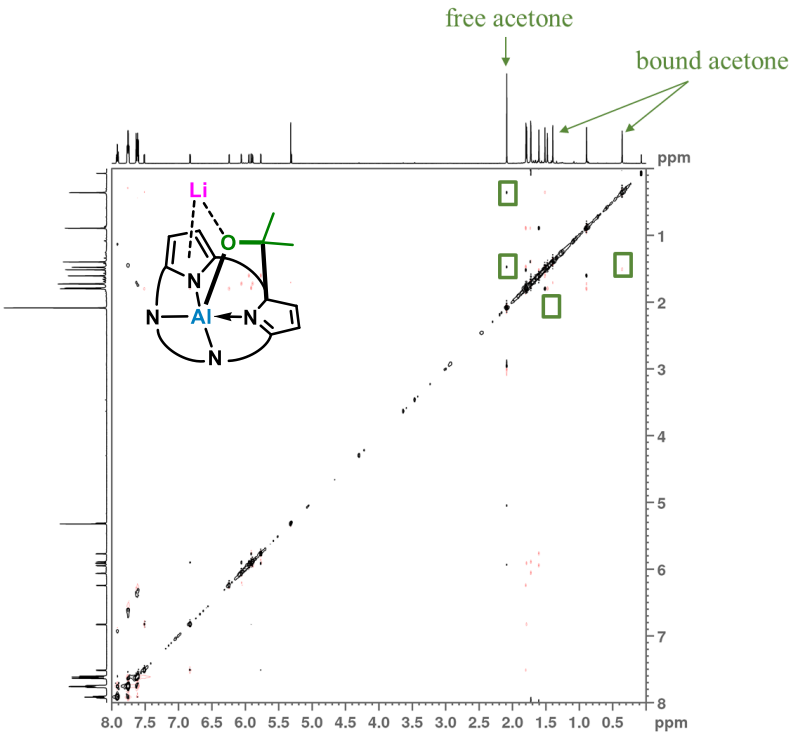


Figure S 19: ^{1}H ^{1}H NOESY NMR (600 MHz, DCM-d_2, 295 K, τ_m = 300 ms) spectra of 1,2 bound [Li][**1***-acetone] exhibiting negligible exchange between bound and free acetone.

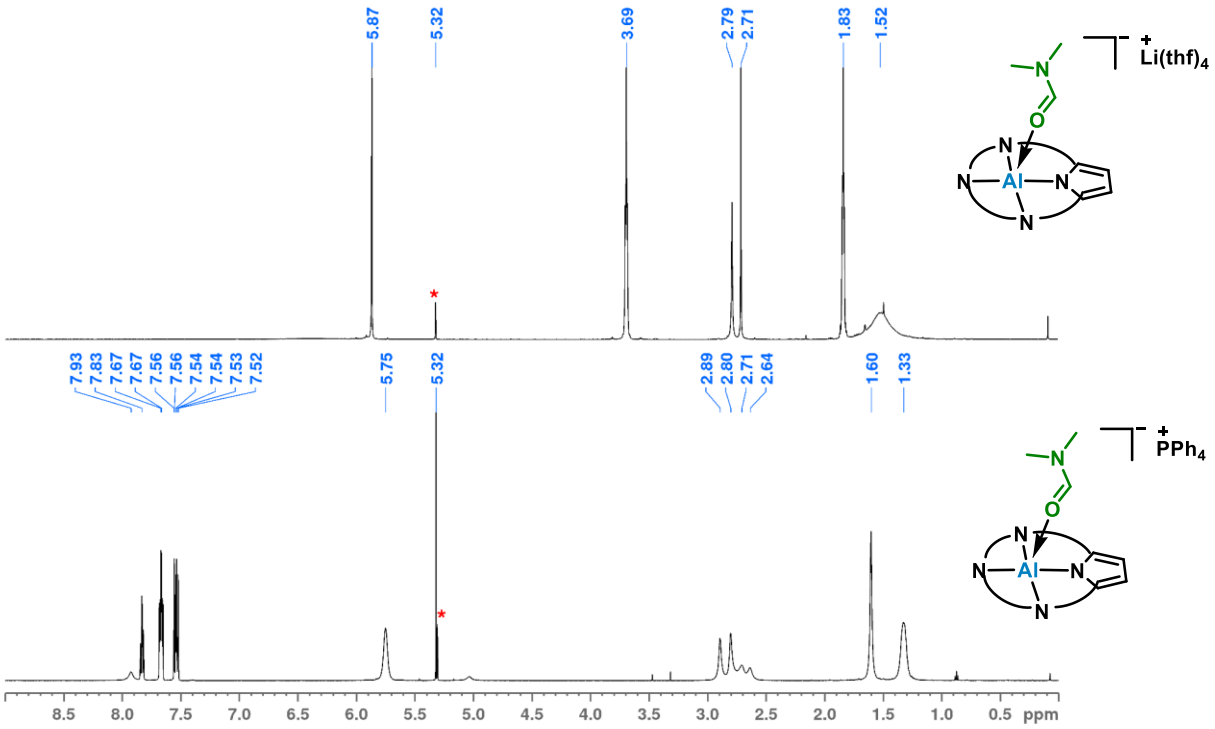


Figure S 20: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectra of σ-coordinated [PPh_4][**1**-dimethylformamide] and σ-coordinated [$Li(thf)_4$][**1**-dimethylformamide], demonstrating the limitation of the controlling of the coordination mode.

7.2. **Reversibility of coordination mode**

The reversibility of the coordination of $[Li]^+$ to control the binding mode of the substrates were investigated and are exemplarily shown for cyclopentanone changing from $[Li(thf)_2]$[**1***-cyclopentanone] to $[Li(12crown4)(thf)_2]$[**1**-cyclopentanone] and back to $[Li(thf)_2]$[**1***-cyclopentanone] by subsequently conducted additions of excesses of [12]crown-4 or LiI (see fig. S 20).

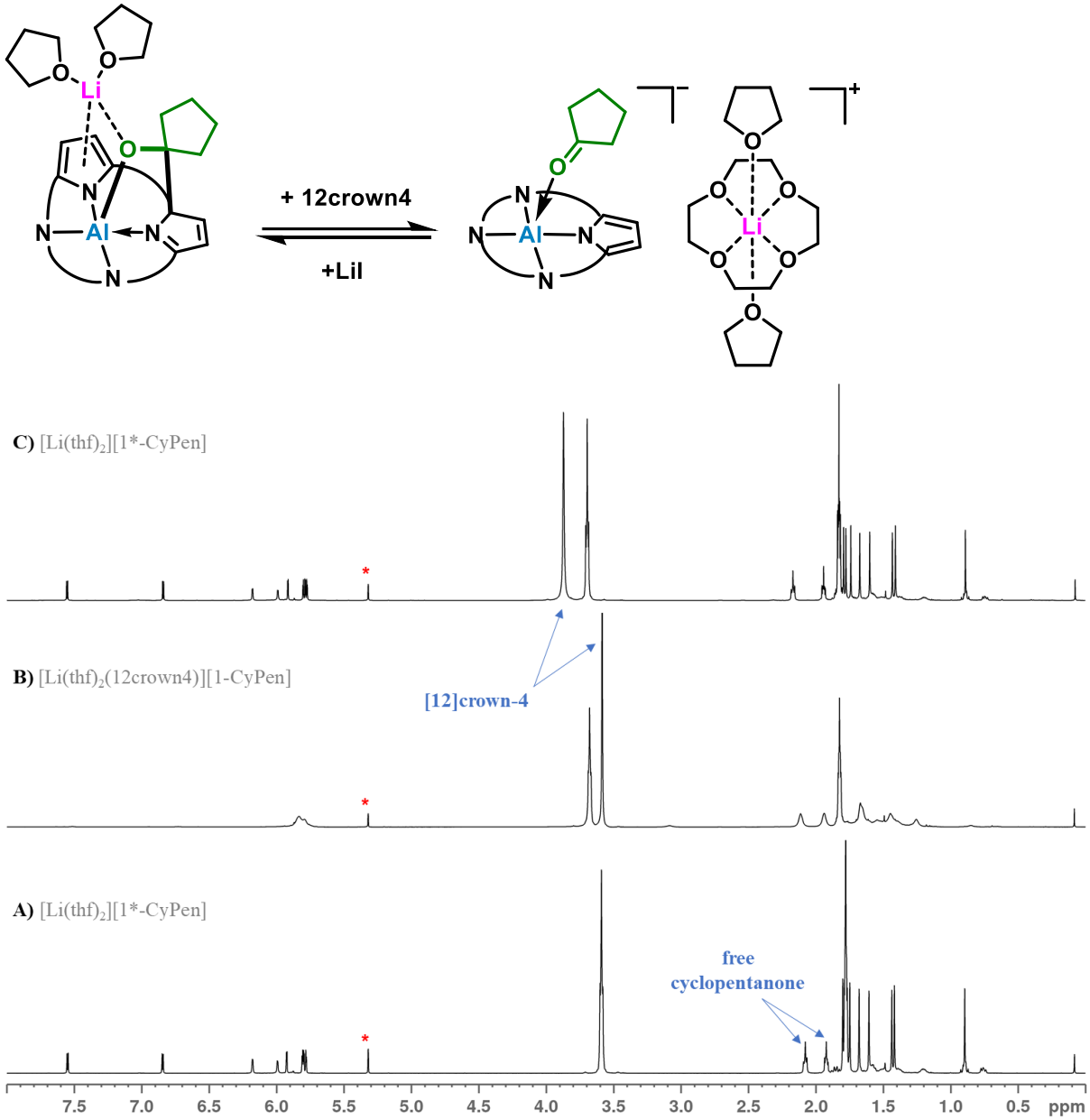


Figure S 21: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectra of A) $[Li(thf)_2]$[**1***-cyclopentanone], B) after addition of [12]crown-4 giving rise of [Li([12]crown-4)$(thf)_2$][**1**-cyclopentanone] and C) after further addition of LiI obtaining $[Li(thf)_2]$[**1***-cyclopentanone] again.

8. Substrate exchange experiments

This section sketches the conducted exchange experiments between various adducts and various substrates listed in table S 2. All starting adducts were freshly prepared and subjected to the substrate of interest at rt. If no exchange occurred at rt the solution was heated up to 70 °C for the stated time to study the behavior at elevated temperature.

Table S 2: Scope of the exchange experiments performed in the given solvent at room temperature. Observed coordination mode of each substrate is given and the occurrence of the exchange marked with yes (y) or no (n).

	solvent	adduct sub-strate	coordination before exchange	exchange substrate	exchange proceed	coordination af-ter exchange	figure
[Li][**1**]	thf	*p*Me-BA	1,2	*p*NO_2-BA	y	1,2	S 22
[Li][**1**]	thf	CO_2	1,2	*p*NO_2-BA	y	1,2	S 23/24
[Li][**1**]	thf	CO_2	1,2	*p*DMA-BA	y[a]	-	S 25/26
[Li][**1**]	thf	CO_2	1,2	CyA	y[a]	-	S27/28
[Li][**1**]	thf	CO_2	1,2	CyPen	n	-	S 29/30
[Li][**1**]	thf	CO_2	1,2	*p*Me-BA	y[a]	-	S 31/32
[Li][**1**]	thf	CO_2	1,2	acetone	n	-	S 33/34
[Li][**1**]	dcm	acetone	1,2	*p*DMA-BA	y	1,2	S 35
[Li][**1**]	dcm	*p*DMA-BA	1,2	CyA	y	1,2	S 36
[PPh_4][**1**]	dcm	acetone	σ	*p*DMA-BA	y	σ	S 37
[PPh_4][**1**]	dcm	*p*DMA-BA	σ	CyA	y	1,2	S 38
[PPh_4][**1**]	dcm	*p*Me-BA	1,2	CyA	y[b]	1,2	S 39
[Li][**1**]	dcm	*p*DMA-BA	1,2	*p*M-BA	y	1,2	S 40

[a]exchange proceed at a higher temperature
[b]equilibrium occurred

The green asterisk marks free substrate or substrate in excess. The red asterisk marks the solvent residual signal. Characteristic peaks indicating the exchange are marked and followed with blue arrows.

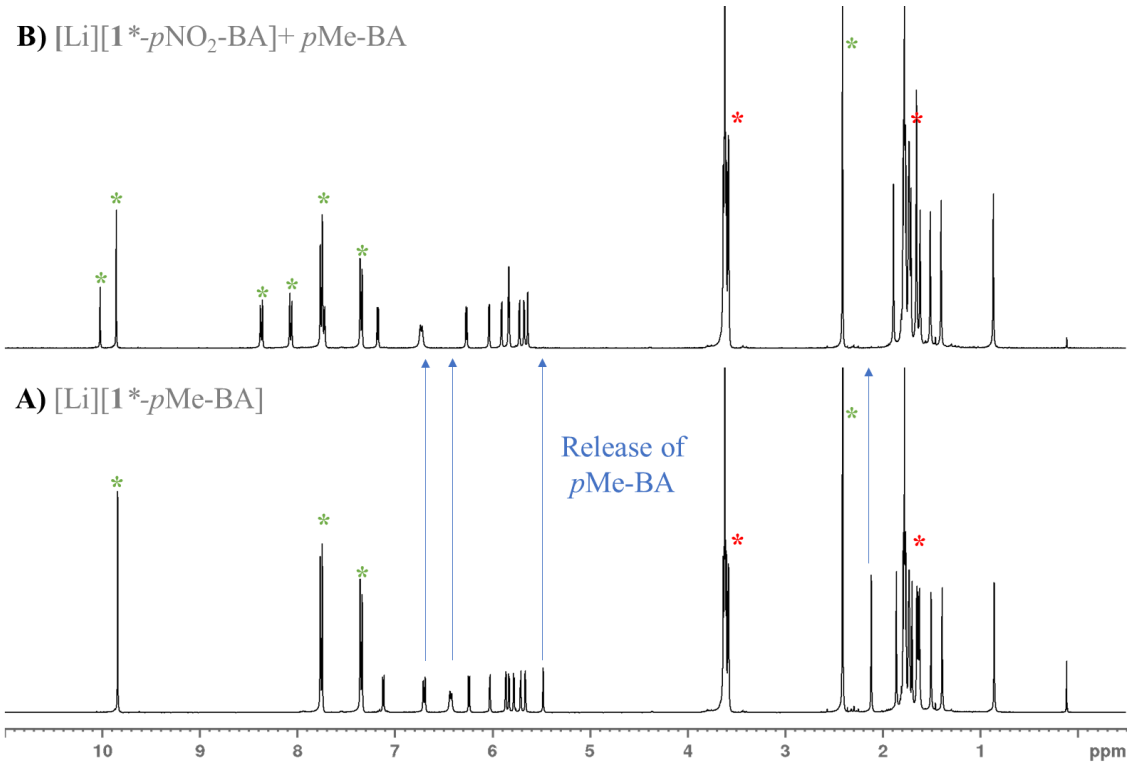


Figure S 22: Exchange of *p*Me-BA against *p*NO_2-BA in THF-d_8 at room temperature at [Li][**1**] followed by ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K) from A) to B). The spectra were measured directly after the addition of the substrates.

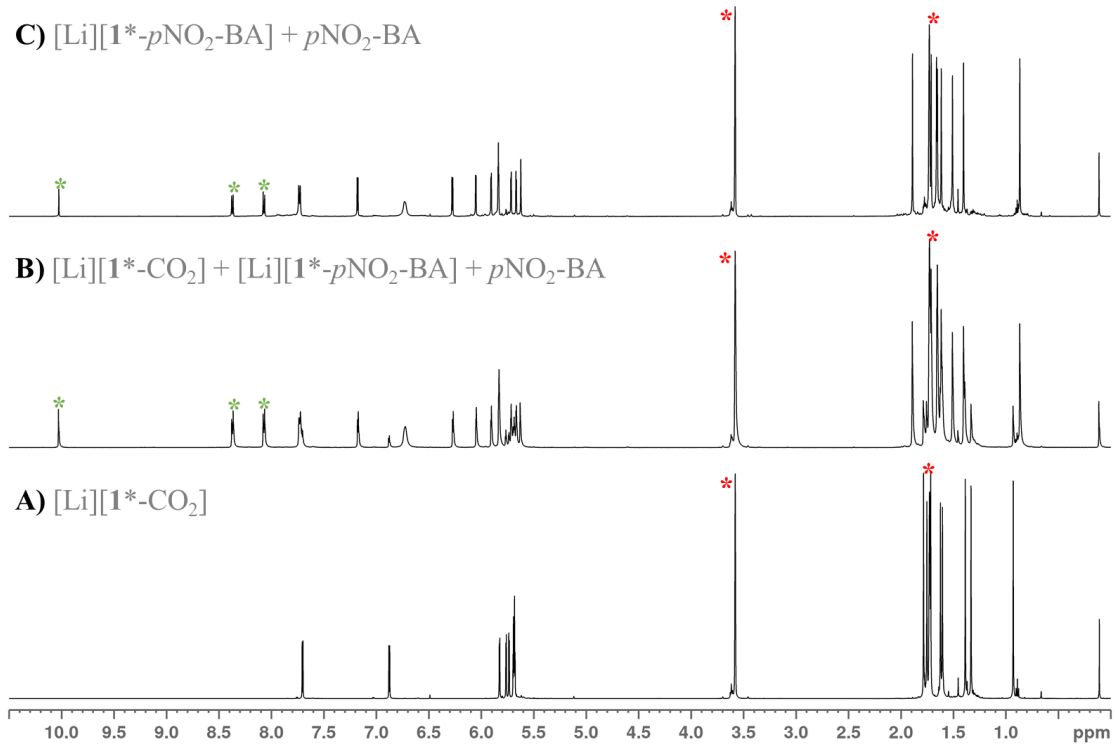


Figure S 23: Exchange of CO_2 against *p*NO_2-BA in THF-d_8 at room temperature at [Li][**1**] followed by ^{1}H NMR spectroscopy (600 MHz, THF-d_8, 295 K) from A) showing the pure CO_2 adduct, to B) after three hours at rt showing both adducts, to C) after two days showing full conversion to the *p*NO_2-BA adduct.

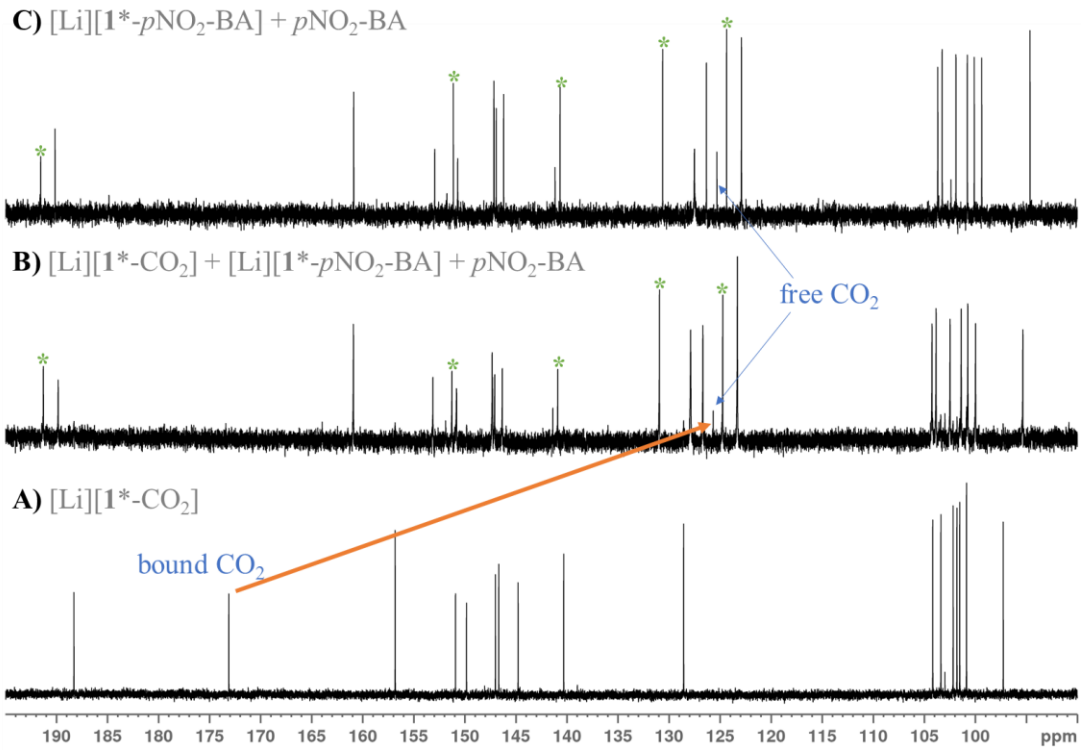


Figure S 24: Exchange of CO_2 against *p*NO_2-BA in THF-d_8 at room temperature at [Li][**1**] followed by $^{13}C\{^1H\}$ NMR spectroscopy (150 MHz, THF-d_8, 295 K) from A) showing the pure CO_2 adduct, to B) after three hours at rt showing both adducts, to C) after two days showing full conversion to the *p*NO_2-BA adduct

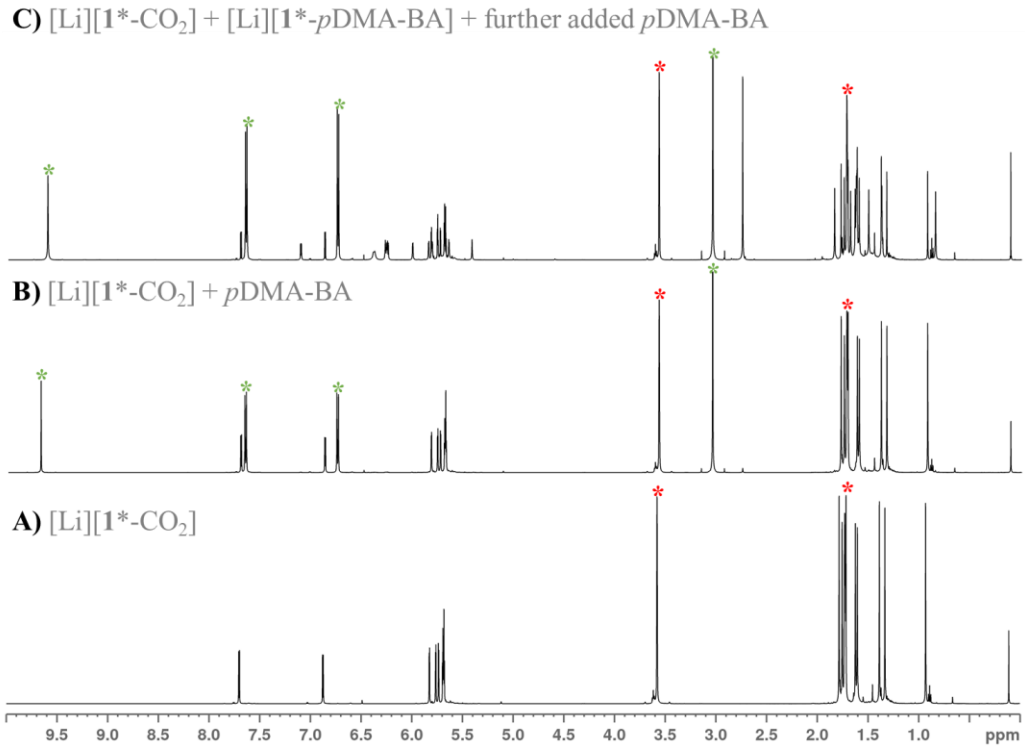


Figure S 25: Exchange of CO_2 against *p*DMA-BA in THF-d_8 at room temperature at [Li][**1**] followed by ^1H NMR spectroscopy (600 MHz, THF-d_8, 295 K) from A) showing the pure CO_2 adduct, to B) after three hours at rt after *p*DMA-BA addition showing no exchange, to C) after 42 h at 70 °C with further addition of *p*DMA-BA showing conversion to a ratio of 1:0.82 of *p*DMA-BA:CO_2.

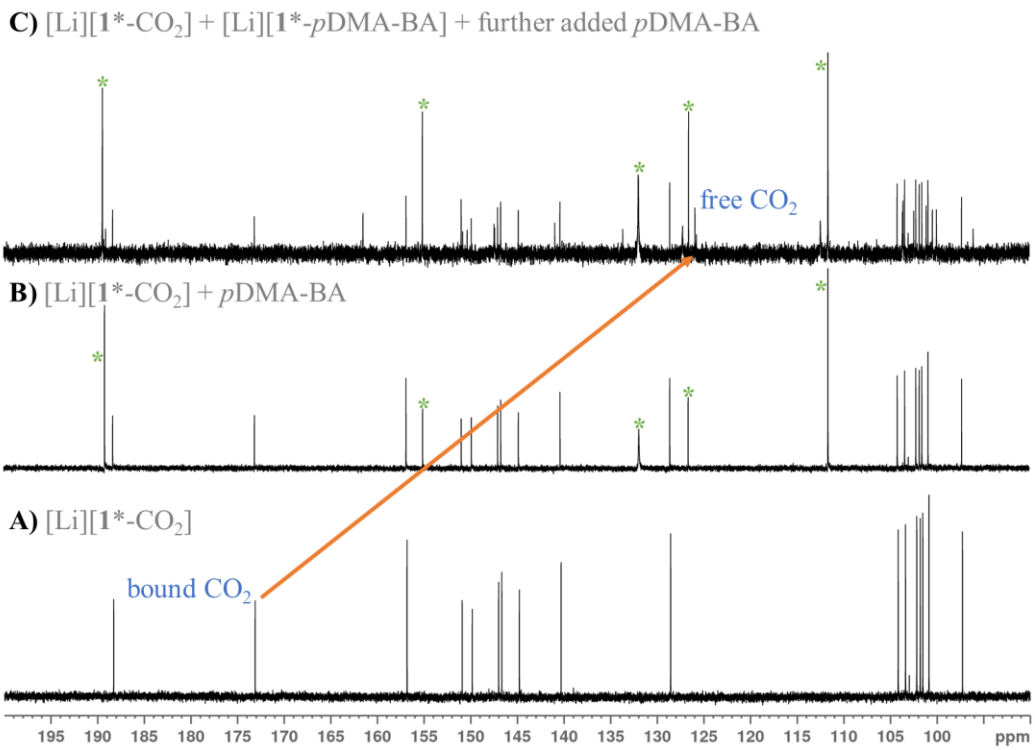


Figure S 26: Exchange of CO_2 against *p*DMA-BA in THF-d_8 at room temperature at [Li][**1**] followed by $^{13}C\{^1H\}$ NMR spectroscopy (150 MHz, THF-d_8, 295 K) from A) showing the pure CO_2 adduct, to B) after three hours at rt after *p*DMA-BA addition showing no exchange, to C) after 42 h at 70 °C with further addition of *p*DMA-BA showing conversion to a ratio of 1:0.82 of *p*DMA-BA:CO_2.

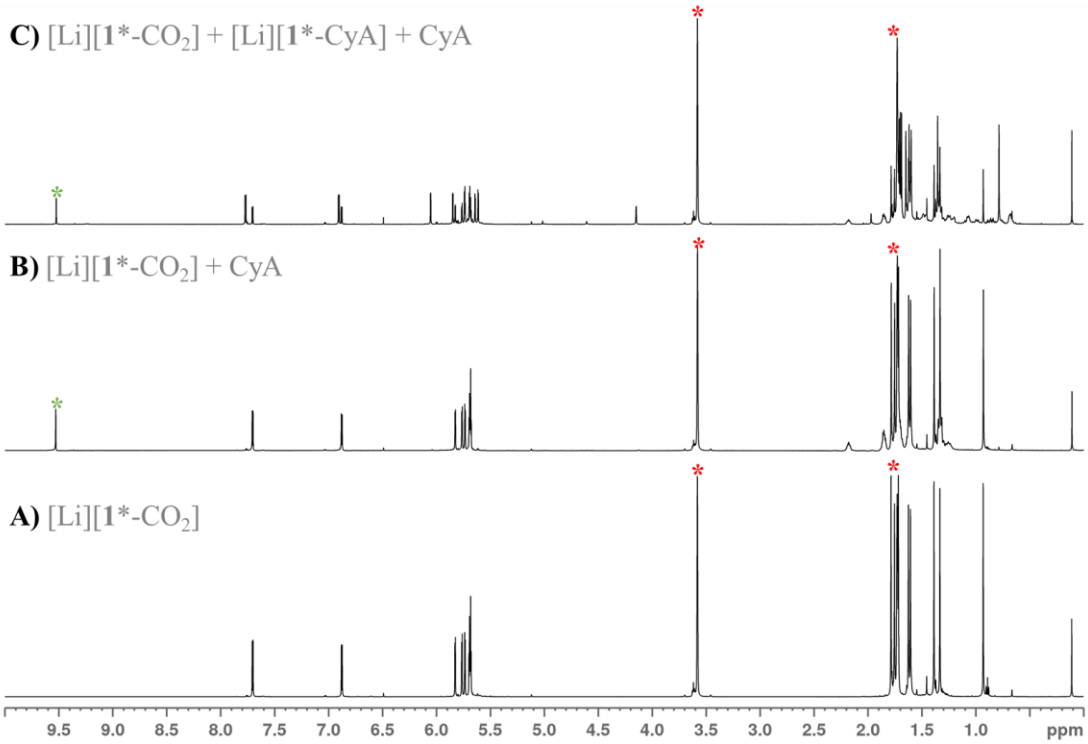


Figure S 27: Exchange of CO_2 against CyA in THF-d_8 at room temperature at [Li][**1**] followed by ^1H NMR spectroscopy (600 MHz, THF-d_8, 295 K) from A) showing the pure CO_2 adduct, to B) after three hours at rt after CyA addition showing no exchange, to C) after 42 h at 70 °C showing conversion to a ratio of 1:0.56 of CyA:CO_2.

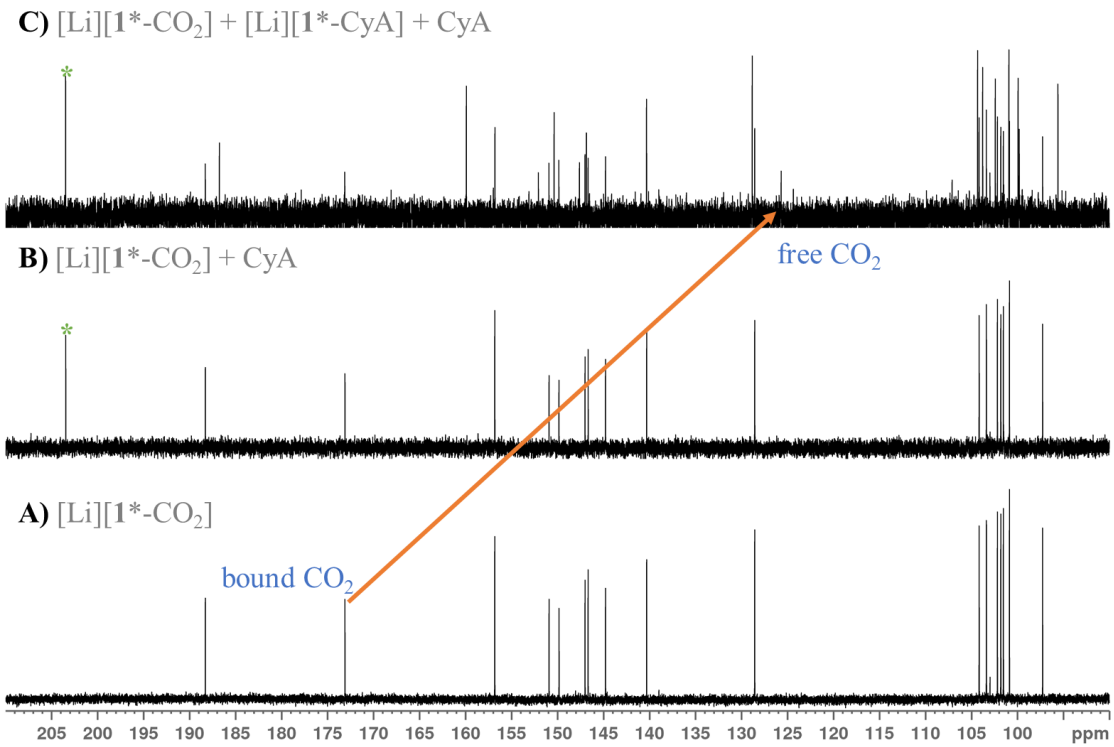


Figure S 28: Exchange of CO_2 against CyA in THF-d_8 at room temperature at [Li][**1**] followed by $^{13}C\{^1H\}$ NMR spectroscopy (150 MHz, THF-d_8, 295 K) from A) showing the pure CO_2 adduct, to B) after three hours at rt after CyA addition showing no exchange, to C) after 42 h at 70 °C showing conversion to a ratio of 1:0.56 of CyA:CO_2.

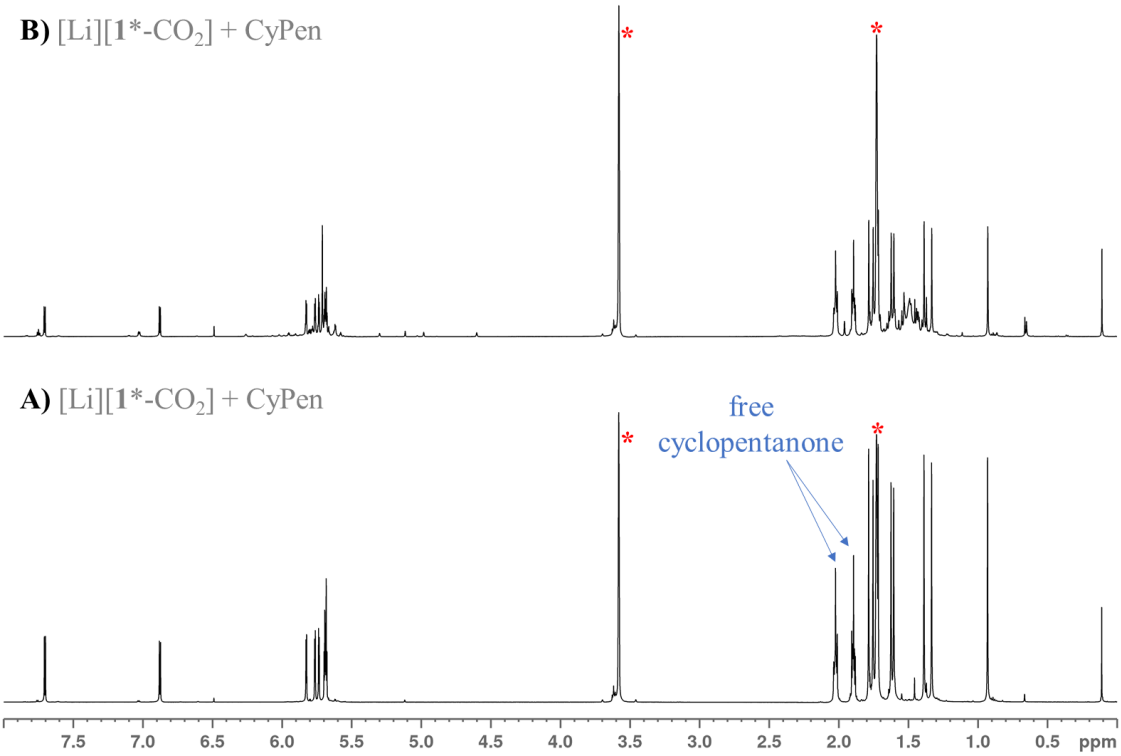


Figure S 29: Exchange of CO_2 against CyPent in THF-d_8 at room temperature at [Li][**1**] followed by ^1H NMR spectroscopy (600 MHz, THF-d_8, 295 K) from A) showing the CO_2 adduct at rt in presence of CyPen, to B) after 42 h at 70 °C showing no conversion.

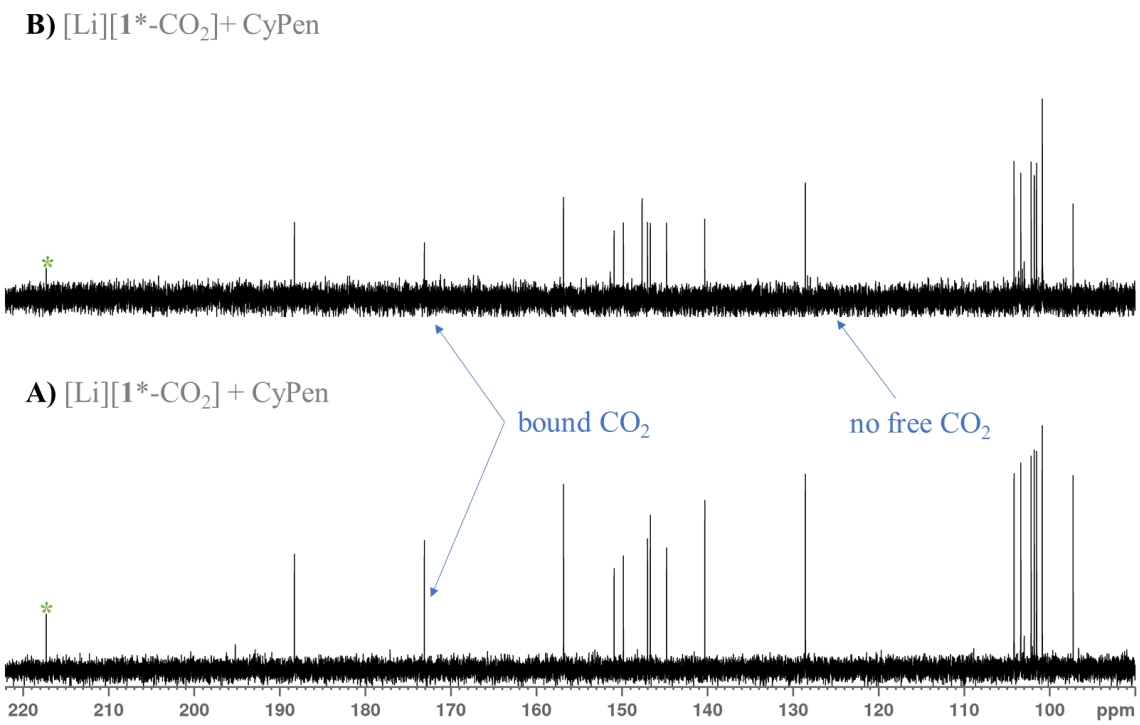


Figure S 30: Exchange of CO_2 against CyPent in THF-d_8 at room temperature at [Li][**1**] followed by $^{13}C\{^1H\}$ NMR spectroscopy (150 MHz, THF-d_8, 295 K) from A) showing the CO_2 adduct at rt in presence of CyPen, to B) after 42 h at 70 °C showing no conversion.

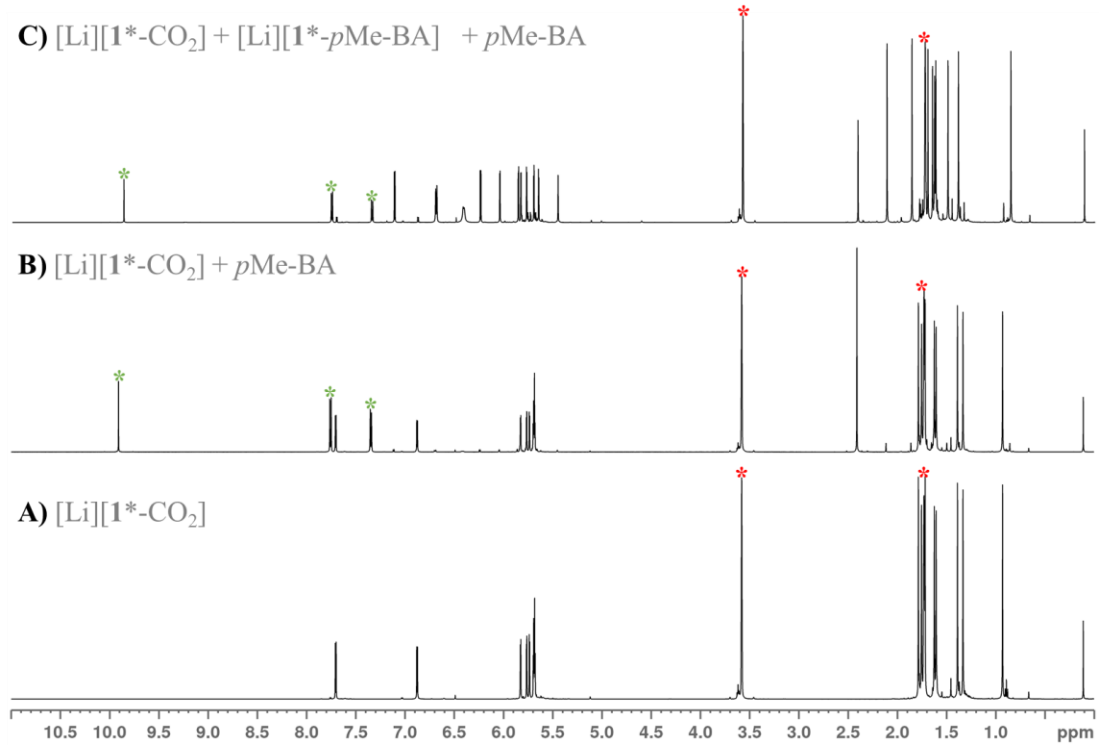


Figure S 31: Exchange of CO_2 against *p*Me-BA in THF-d_8 at room temperature at [Li][**1**] followed by ^1H NMR spectroscopy (600 MHz, THF-d_8, 295 K) from A) showing the pure CO_2 adduct, to B) after three hours at rt after *p*Me-BA addition showing traces of exchange to C) after 29 h at 70 °C showing conversion to a ratio of 1:0.11 of *p*Me-BA:CO_2.

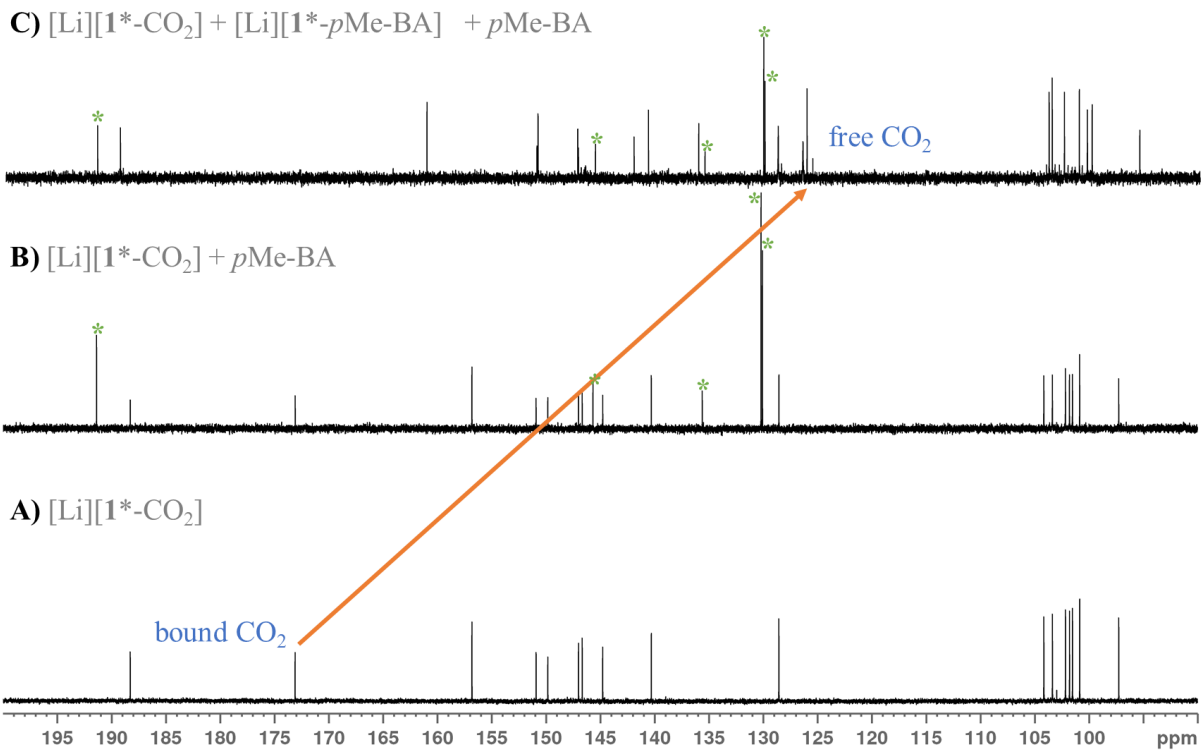


Figure S 32: Exchange of CO_2 against *p*Me-BA in THF-d_8 at room temperature at [Li][**1**] followed by $^{13}C\{^1H\}$ NMR spectroscopy (150 MHz, THF-d_8, 295 K) from A) showing the pure CO_2 adduct, to B) after three hours at rt after *p*Me-BA addition showing traces of exchange, to C) after 29 h at 70 °C showing conversion to a ratio of 1:0.11 of *p*Me-BA:CO_2.

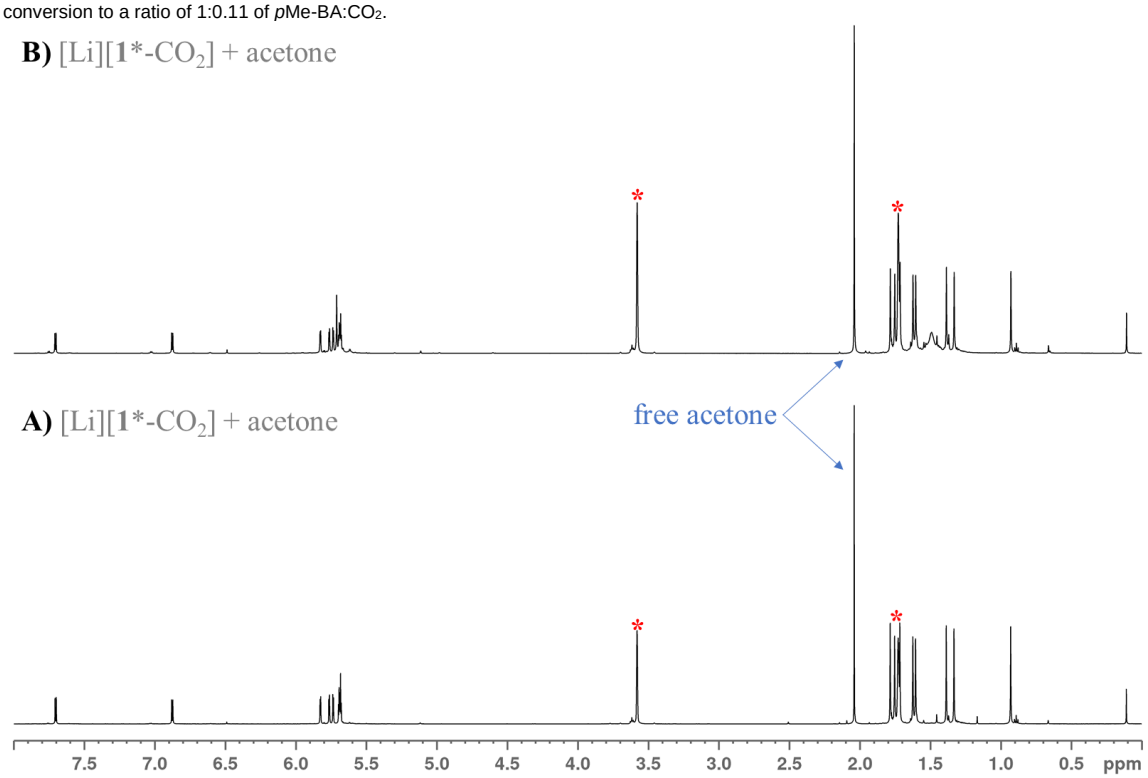


Figure S 33: Exchange of CO_2 against acetone in THF-d_8 at room temperature at [Li][**1**] followed by ^1H NMR spectroscopy (600 MHz, THF-d_8, 295 K) from A) showing the CO_2 adduct in presence of acetone at rt to B) after 34 h at 70 °C showing no replacement of CO_2.

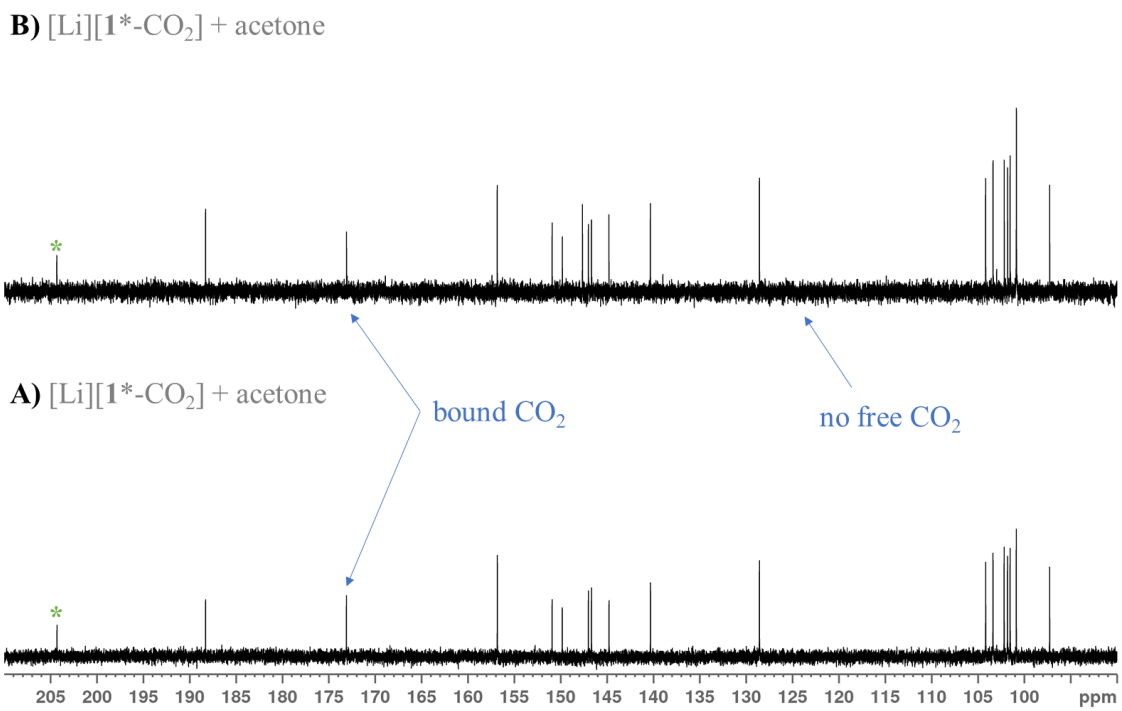


Figure S 34: Exchange of CO_2 against acetone in THF-d_8 at room temperature at [Li][**1**] followed by $^{13}C\{^1H\}$ NMR spectroscopy (150 MHz, THF-d_8, 295 K) from A) showing the CO_2 adduct in presence of acetone at rt, to B) after 34 h at 70 °C showing no replacement of CO_2.

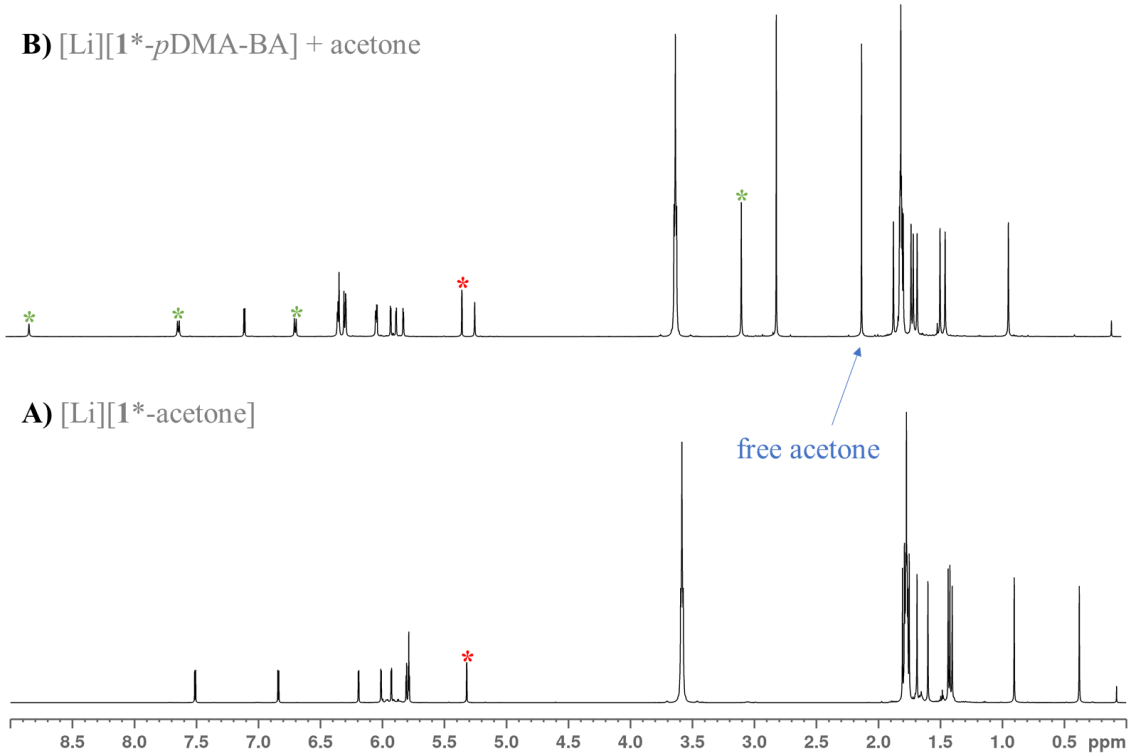


Figure S 35: Exchange of acetone against *p*DMA-BA in DCM-d_2 at room temperature at [Li][**1**] followed by ^1H NMR spectroscopy (600 MHz, DCM-d_2, 295 K) from A) showing the acetone adduct, to B) after addition of *p*DMA-BA at rt showing full conversion to the *p*DMA-BA adduct.

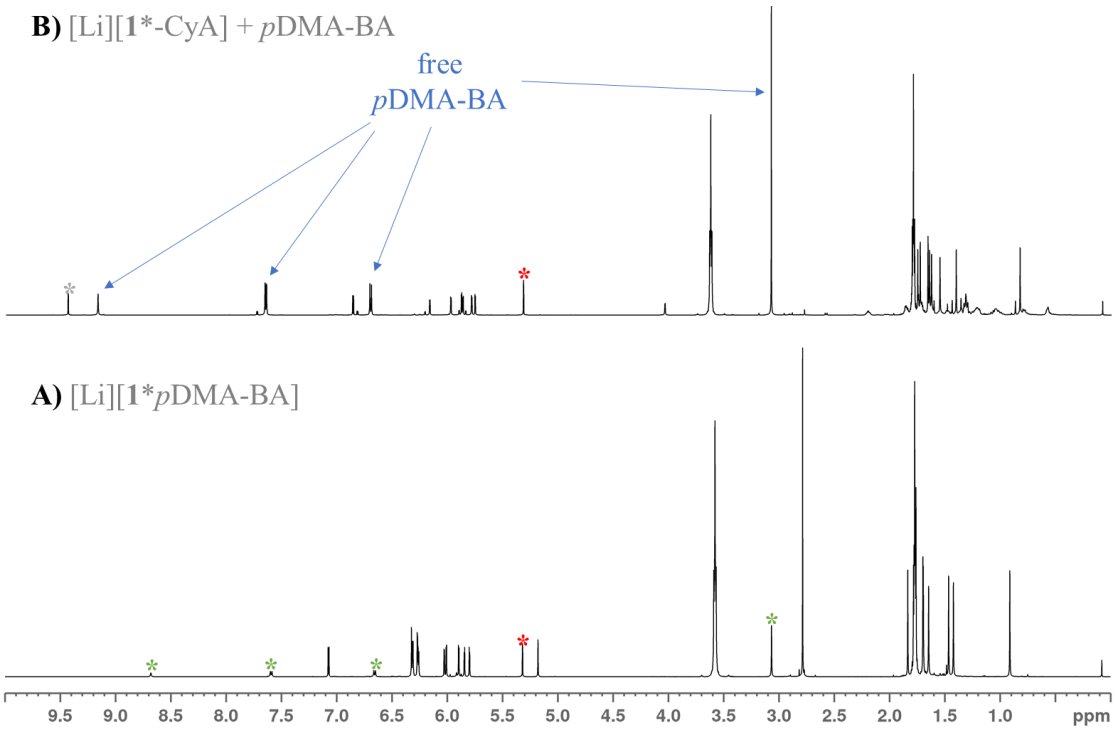


Figure S 36: Exchange of *p*DMA-BA against CyA in DCM-d_2 at room temperature at [Li][**1**] followed by ^{1}H NMR spectroscopy (600 MHz, DCM-d_2, 295 K) from A) showing the *p*DMA-BA adduct, to B) after addition of CyA at rt showing full conversion to the CyA adduct. The grey asterisks mark a small excess of CyA, which is irrelevant for the studied reaction.

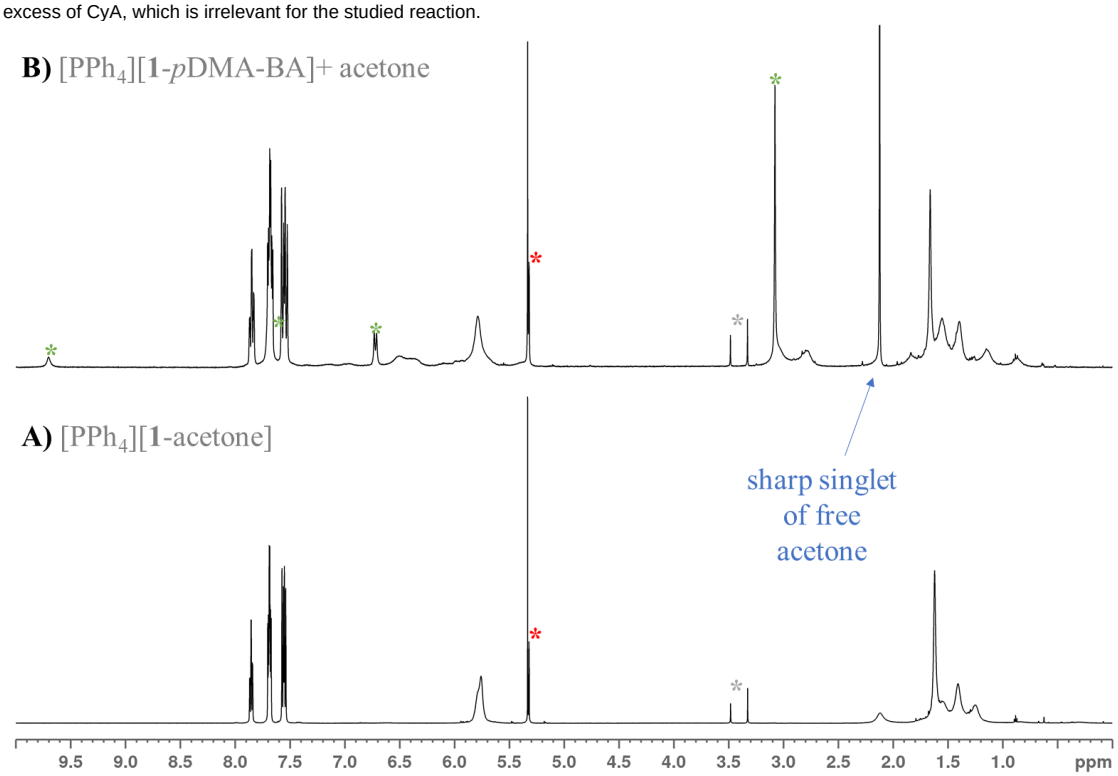


Figure S 37: Exchange of acetone against *p*DMA-BA in DCM-d_2 at room temperature at [PPh_4][**1**] followed by ^{1}H NMR spectroscopy (600 MHz, DCM-d_2, 295 K) from A), showing the acetone adduct, to B), after addition of *p*DMA-BA at rt showing full conversion to the *p*DMA-BA adduct. The gray asterisk indicates present dimethoxyethane, which is irrelevant for the studied reaction.

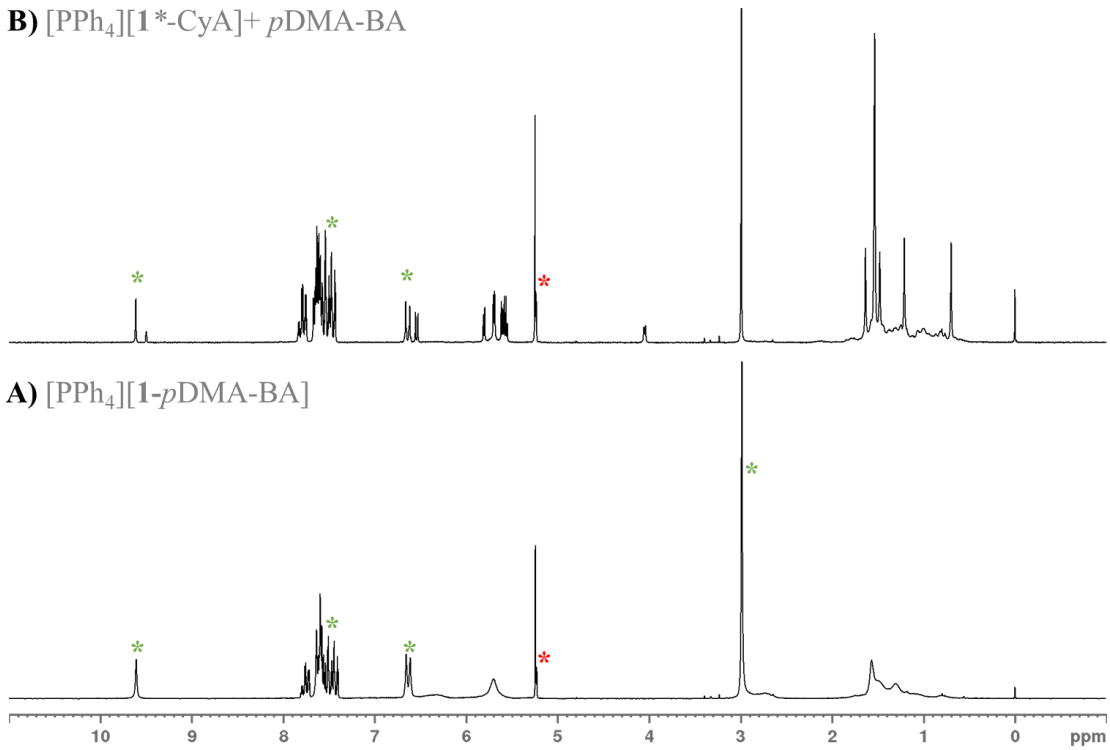


Figure S 38: Exchange of *p*DMA-BA against CyA in DCM-d_2 at room temperature at [PPh_4][**1**] followed by ^{1}H NMR spectroscopy (200 MHz, DCM-d_2, 295 K) from A) showing the *p*DMA-BA adduct, to B) after addition of CyA at rt showing full conversion to the CyA adduct.

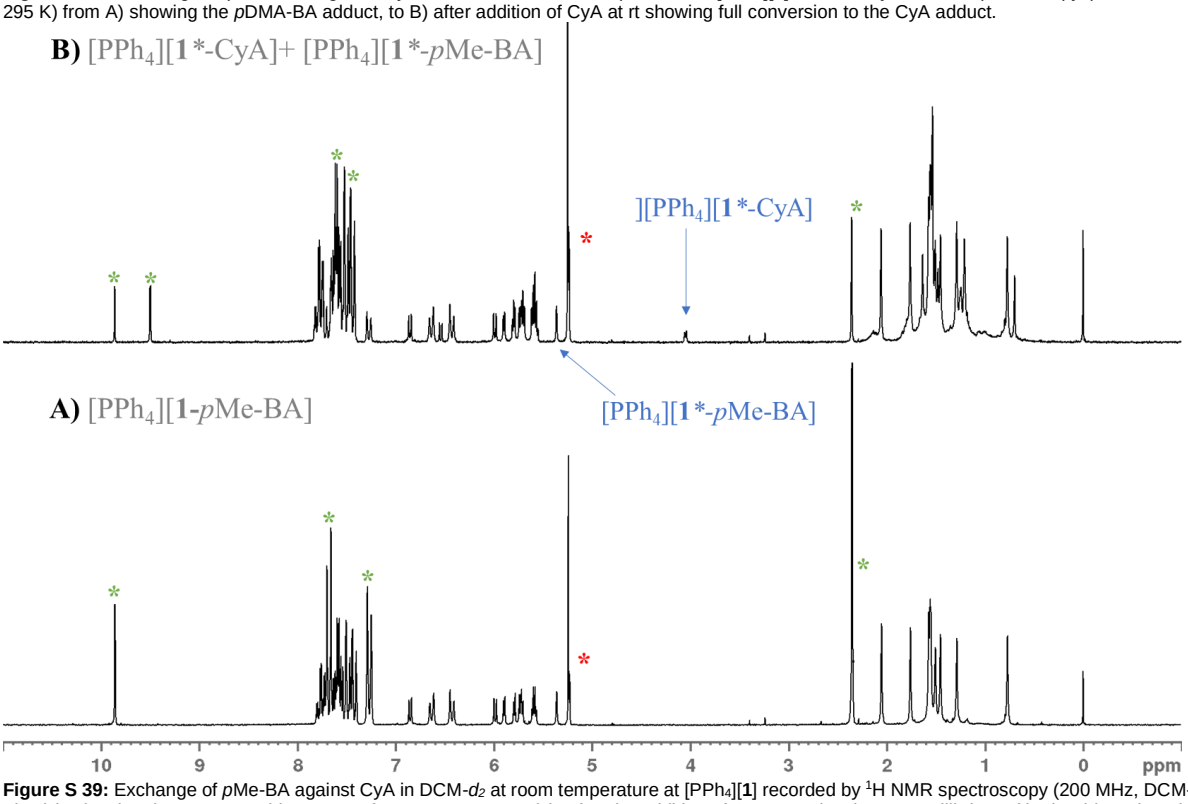


Figure S 39: Exchange of *p*Me-BA against CyA in DCM-d_2 at room temperature at [PPh_4][**1**] recorded by ^{1}H NMR spectroscopy (200 MHz, DCM-d_2, 295 K). A) is showing the *p*Me-BA adduct as a reference spectrum, B) is after the addition of CyA at rt showing an equilibrium of both adducts in ratio 1:0.25 *p*Me-BA:CyA.

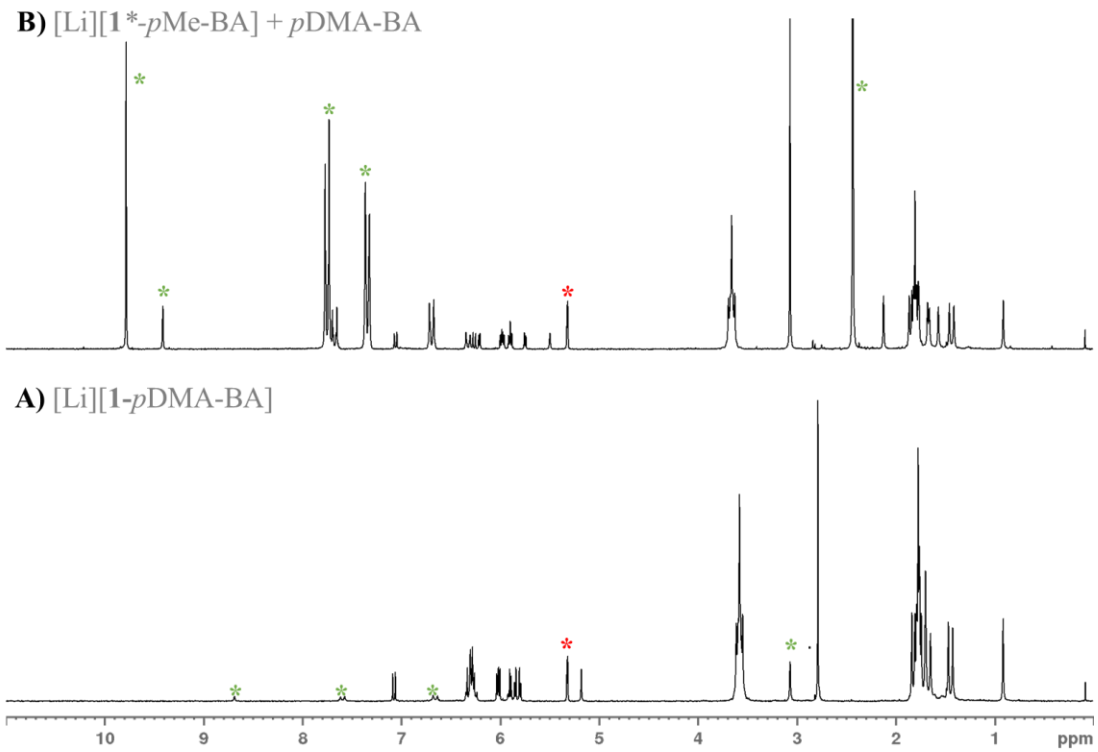


Figure S 40: Exchange of *p*DMA-BA against *p*Me-BA in DCM-d_2 at room temperature at [Li][**1**] studied by ^{1}H NMR spectroscopy (200 MHz, DCM-d_2, 295 K). A) is showing the *p*DMA-BA adduct as a reference spectrum, B) is after the addition of *p*Me-BA at rt showing full exchange to the *p*Me-BA adduct.

9. Hydroboration kinetics

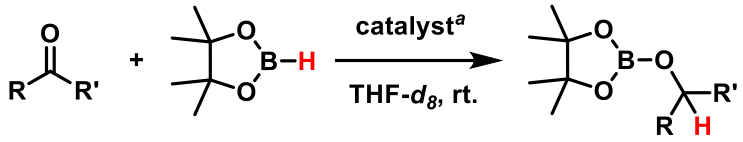


Table S 3: Overview of determined reaction indicators, conditions and reactions.

entry	R	R'	cation	catalyst **1** [mol%]	time [h][b]	TOF [h^{-1}]
1	*p*NMe_2Ph	H	Li	0.05	0.43	> 4500
2	*p*NO_2Ph	H	Li	0.05	19.9	100
3	CH_3	CH_3	Li	0.05	1.01	2000
4	O (CO_2)	-	PPh_4	0.05	24[c]	0.12
5	*p*NMe_2Ph	H	PPh_4	0.05	7.8[d]	90
6	*p*NO_2Ph	H	PPh_4	0.05	38	52
7	CH_3	CH_3	PPh_4	0.05	6.1[e]	45

[a]Hbpin = 0.30 mmol, substrate = 0.10 mmol, 0.6 mL of solvent

[b]time for complete substrate consumption, detected by ^{1}H NMR

[c]time for 3 TON

[d]completeness of reaction 35 %

[e]completeness of reaction 25 %

All reactions were performed under inert gas atmosphere in J.-Young NMR tubes. Due to poor solubility of [PPh_4][**1**] in THF, the stock solution was set up in DCM and added to the reaction mixture in THF. Analysis of the spectra was performed with Dynamics center v.2.5.5 BRUKER software.

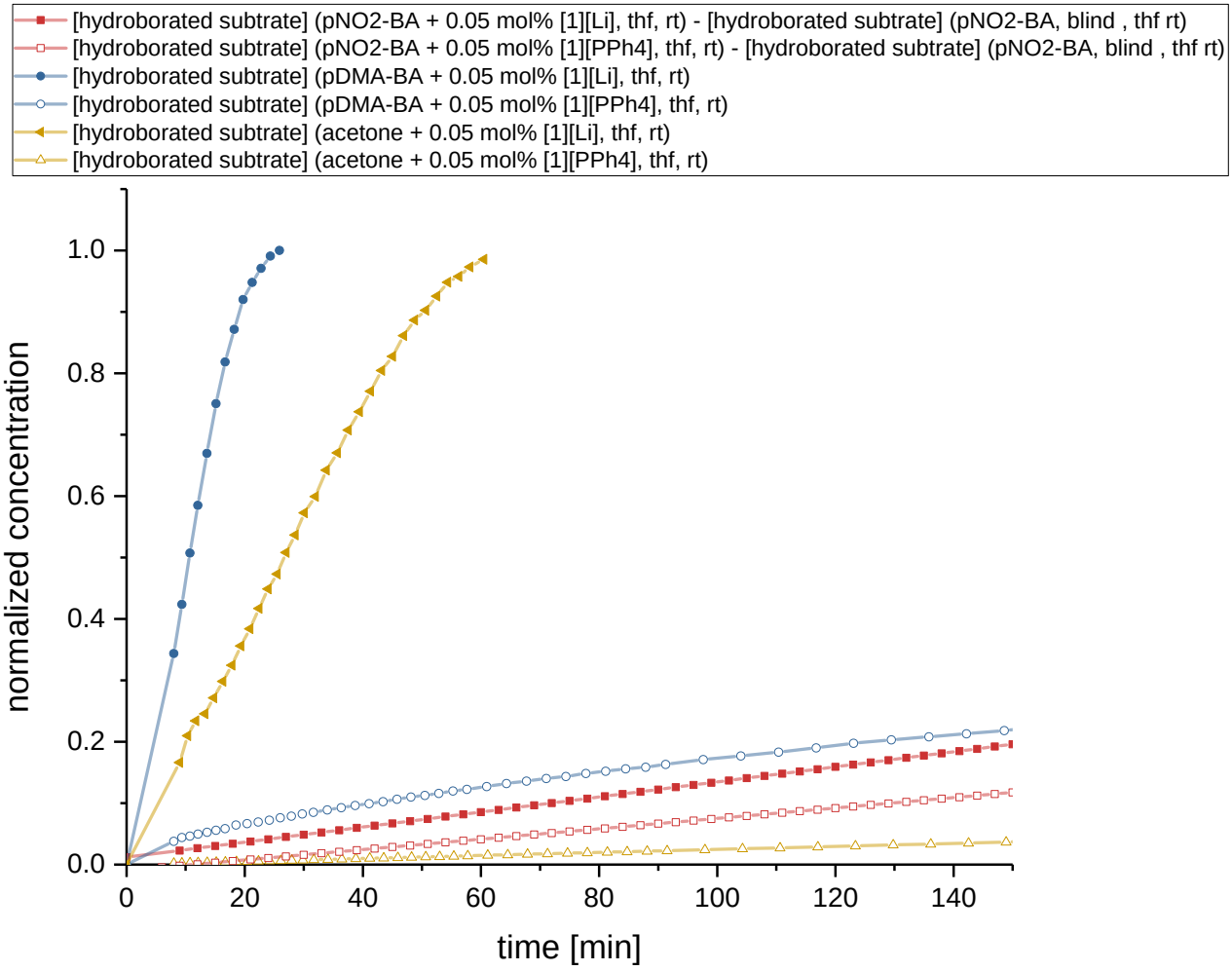


Figure S 41: Concentration profile of hydroboration reactions products with 0.05 mol% [**1**$^-$] as [Li$^+$] or [PPh$_4^+$] salt in thf. Profiles are determined *via* ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K).

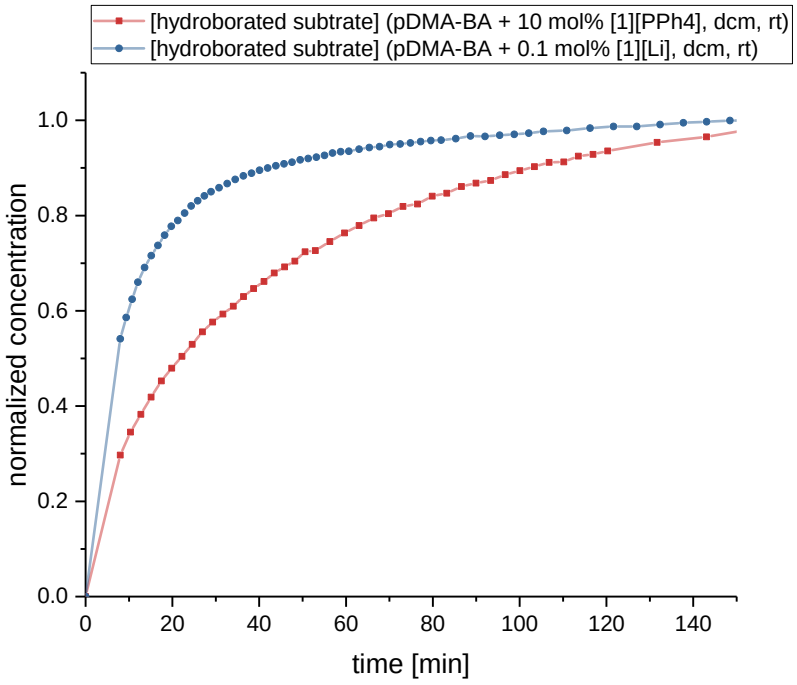


Figure S 42: Concentration profile of hydroboration reaction products of *p*DMA-BA with different concentrations of [**1**$^-$] as [Li$^+$] or [PPh$_4^+$] salt in thf. Profiles are determined *via* ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K).

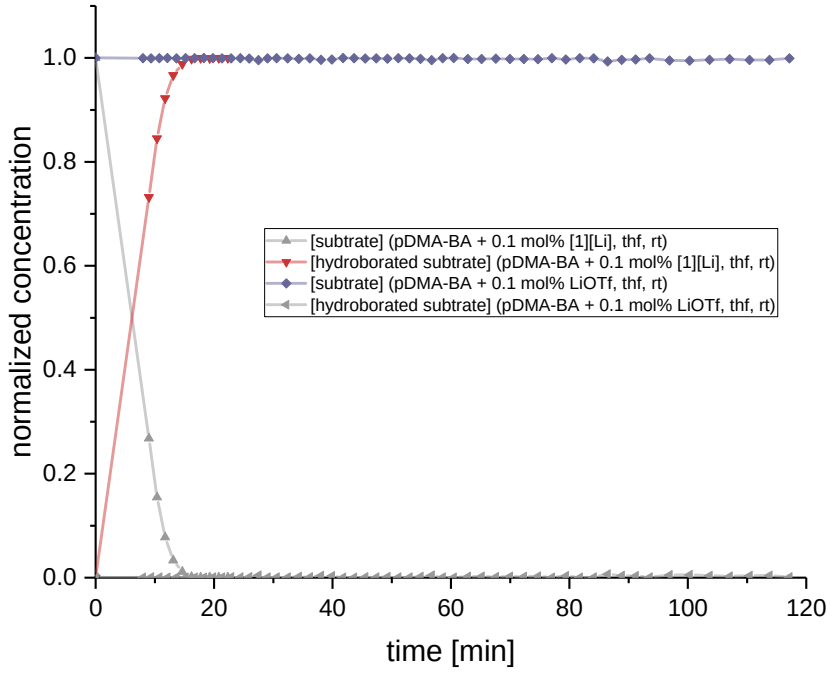


Figure S 43: Concentration profile of hydroboration reaction products of *p*DMA-BA with 0.1 mol% [Li][**1**] and 0.1 mol% [Li][OTf] in thf. Profiles are determined *via* ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K).

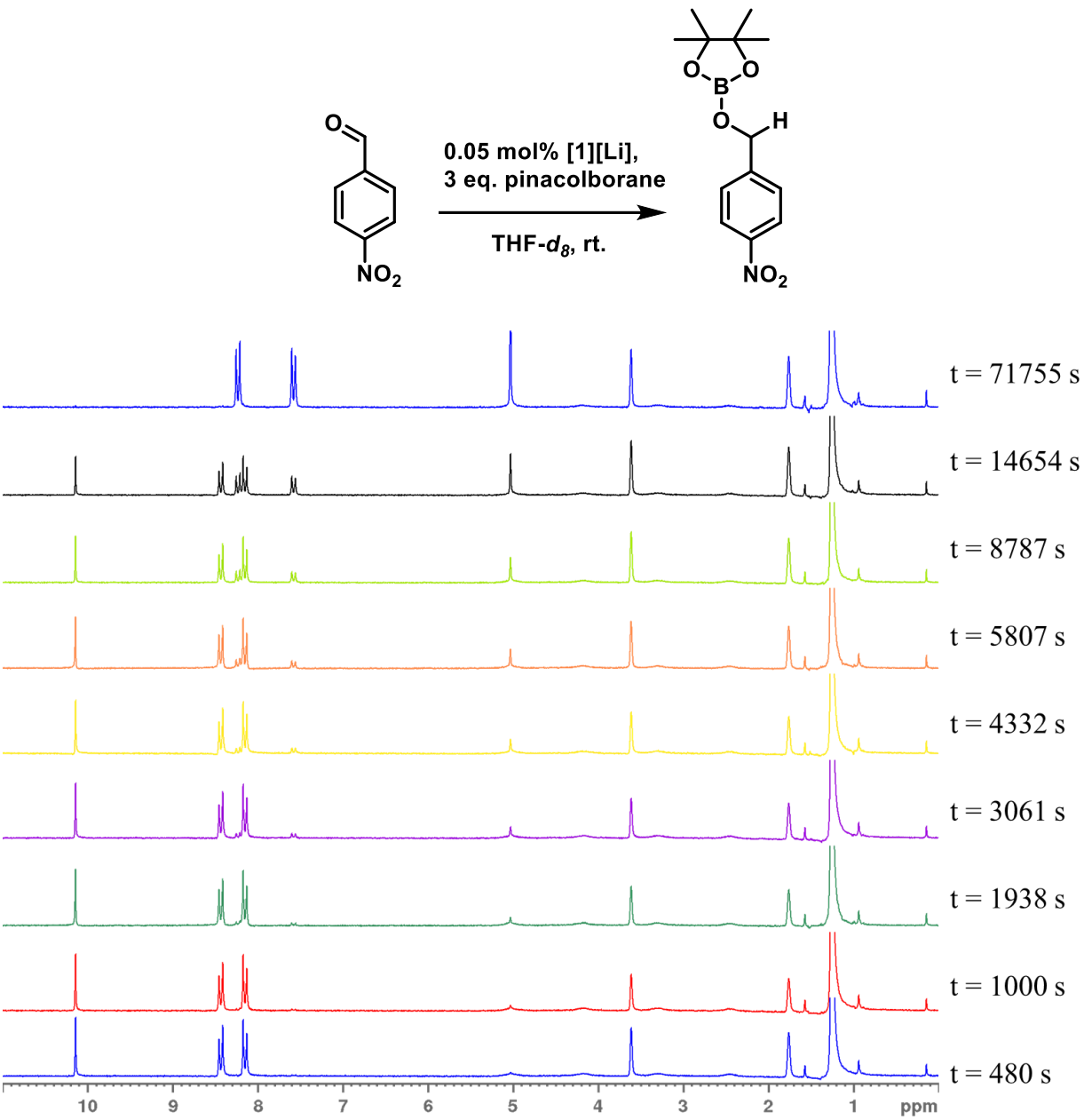


Figure S 44: Hydroboration of *p*NO_2-BA with 0.05 mol% [Li][**1**] followed over time by ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K).

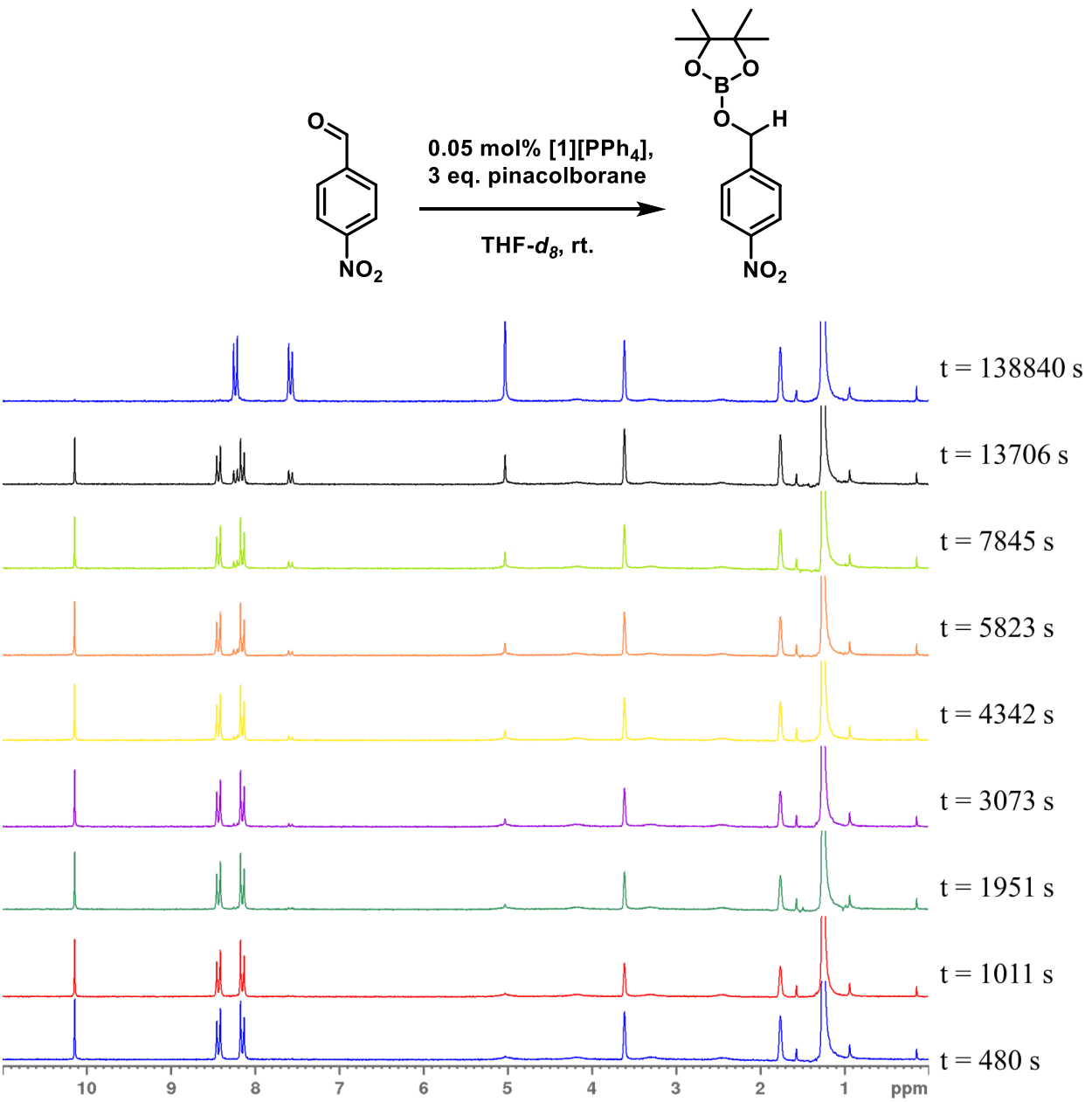


Figure S 45: Hydroboration of *p*NO_2-BA with 0.05 mol% [PPh_4][**1**] followed over time by ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K).

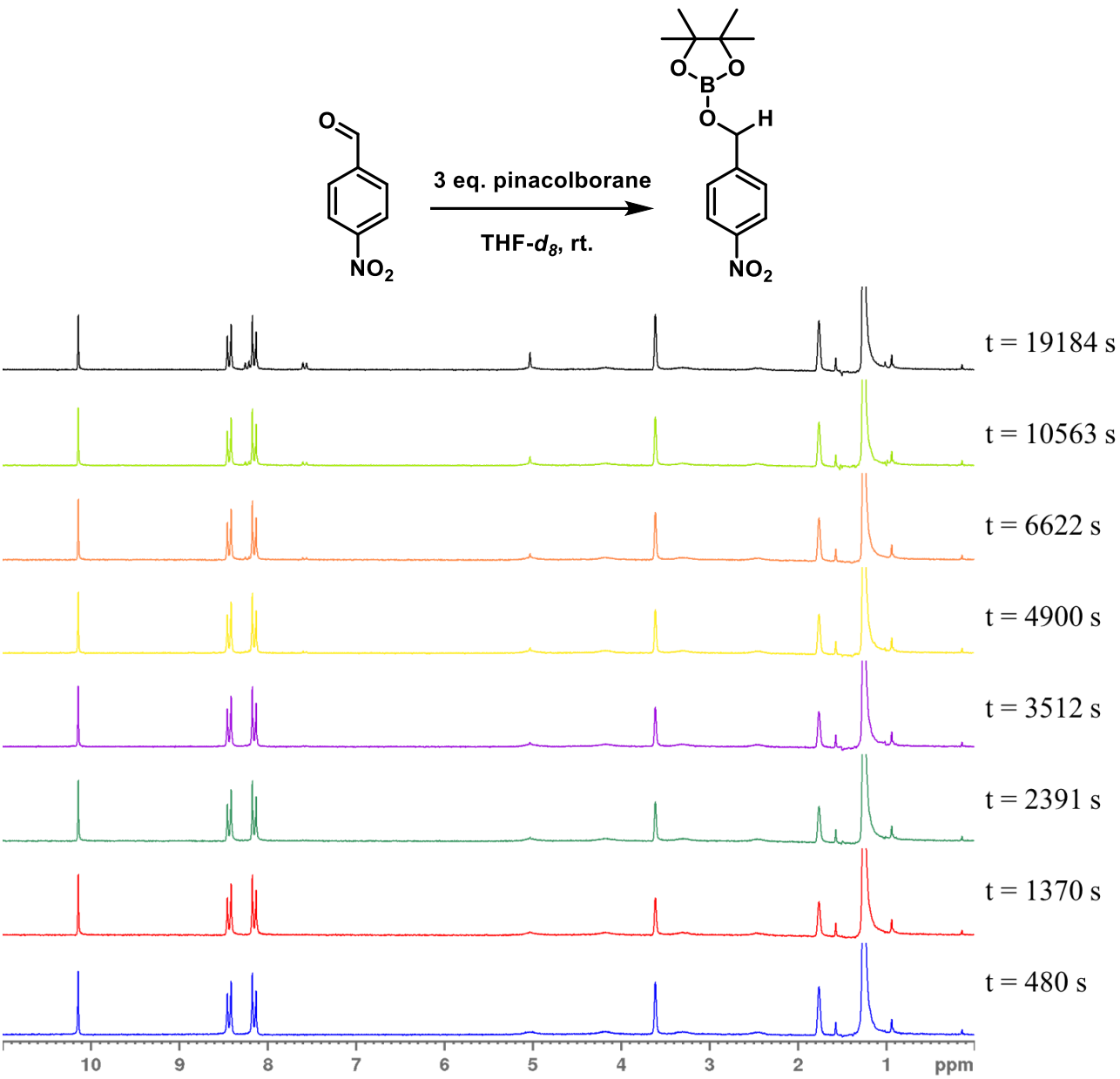


Figure S 46: Self hydroboration of *p*NO_2-BA followed over time by ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K).

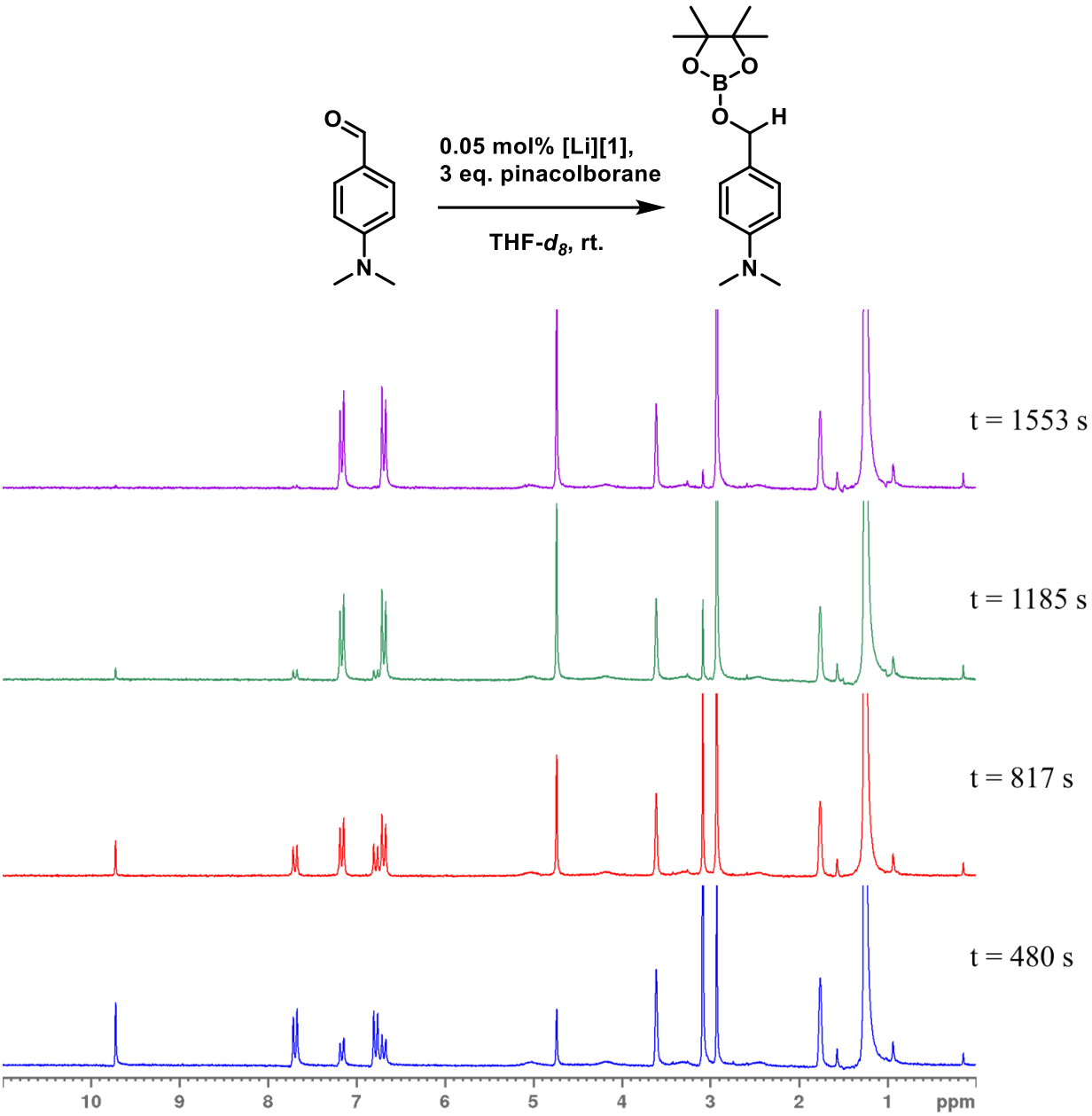


Figure S 47: Hydroboration of *p*DMA-BA with 0.05 mol% [Li][**1**] followed over time by ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K).

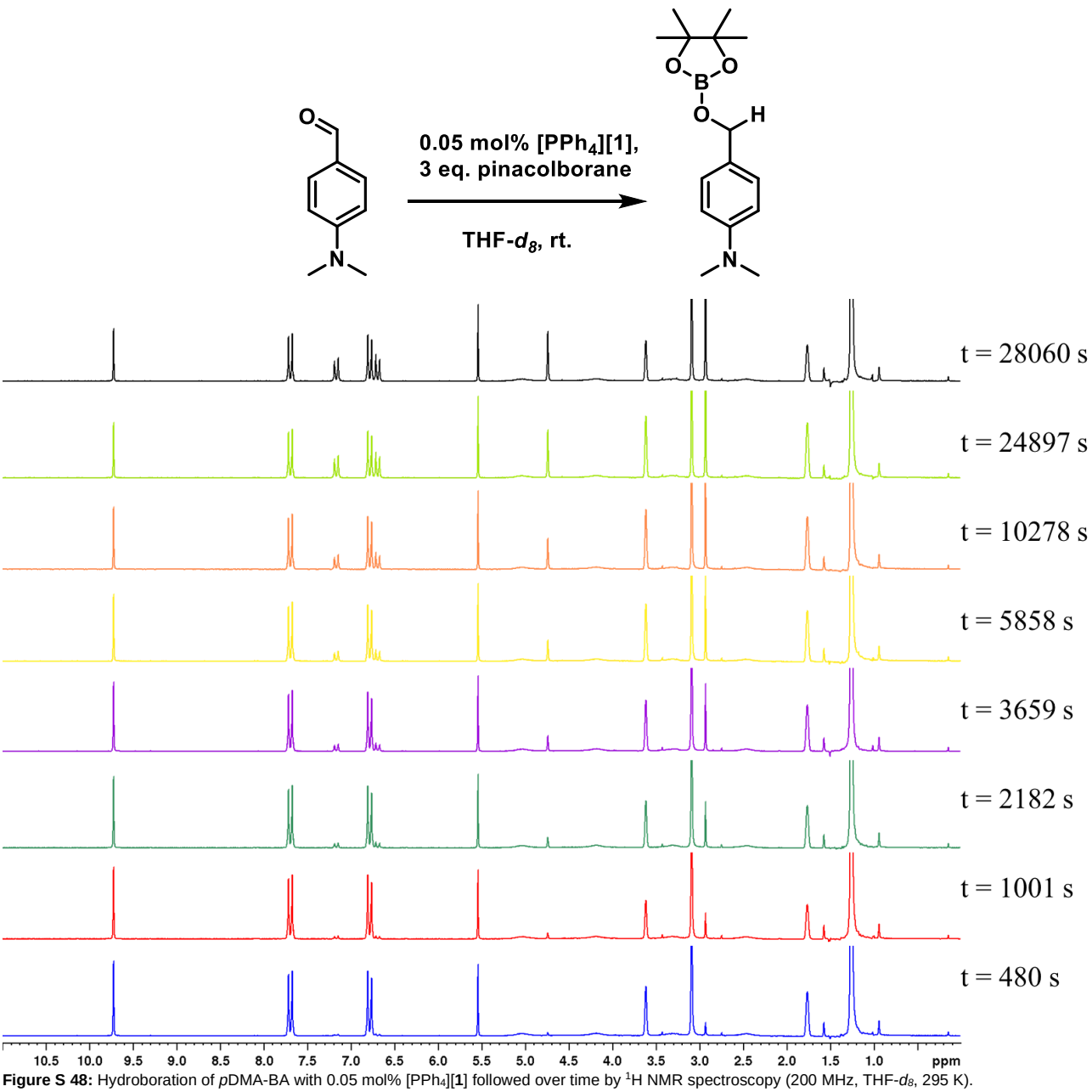


Figure S 48: Hydroboration of *p*DMA-BA with 0.05 mol% [PPh_4][**1**] followed over time by ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K).

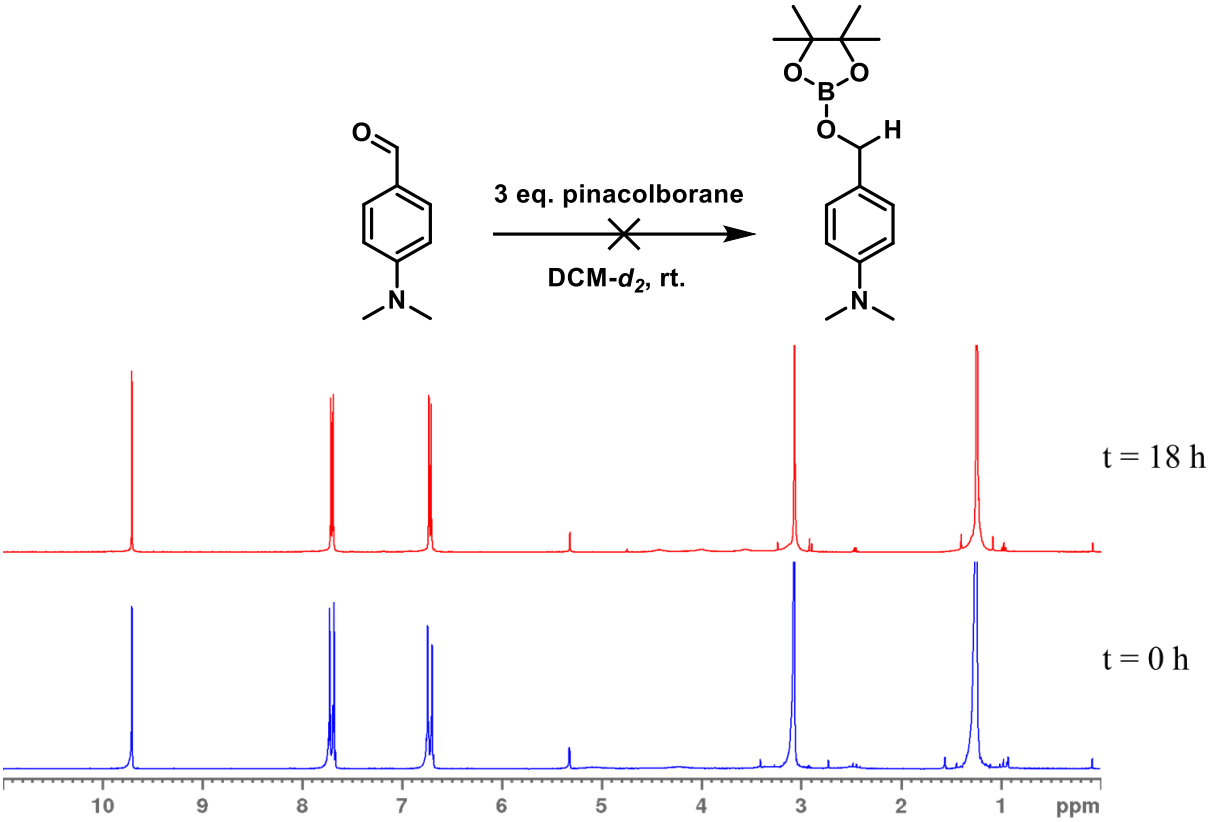


Figure S 49: No reaction between pinacolborane and *p*DMA-BA was detected by ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K).

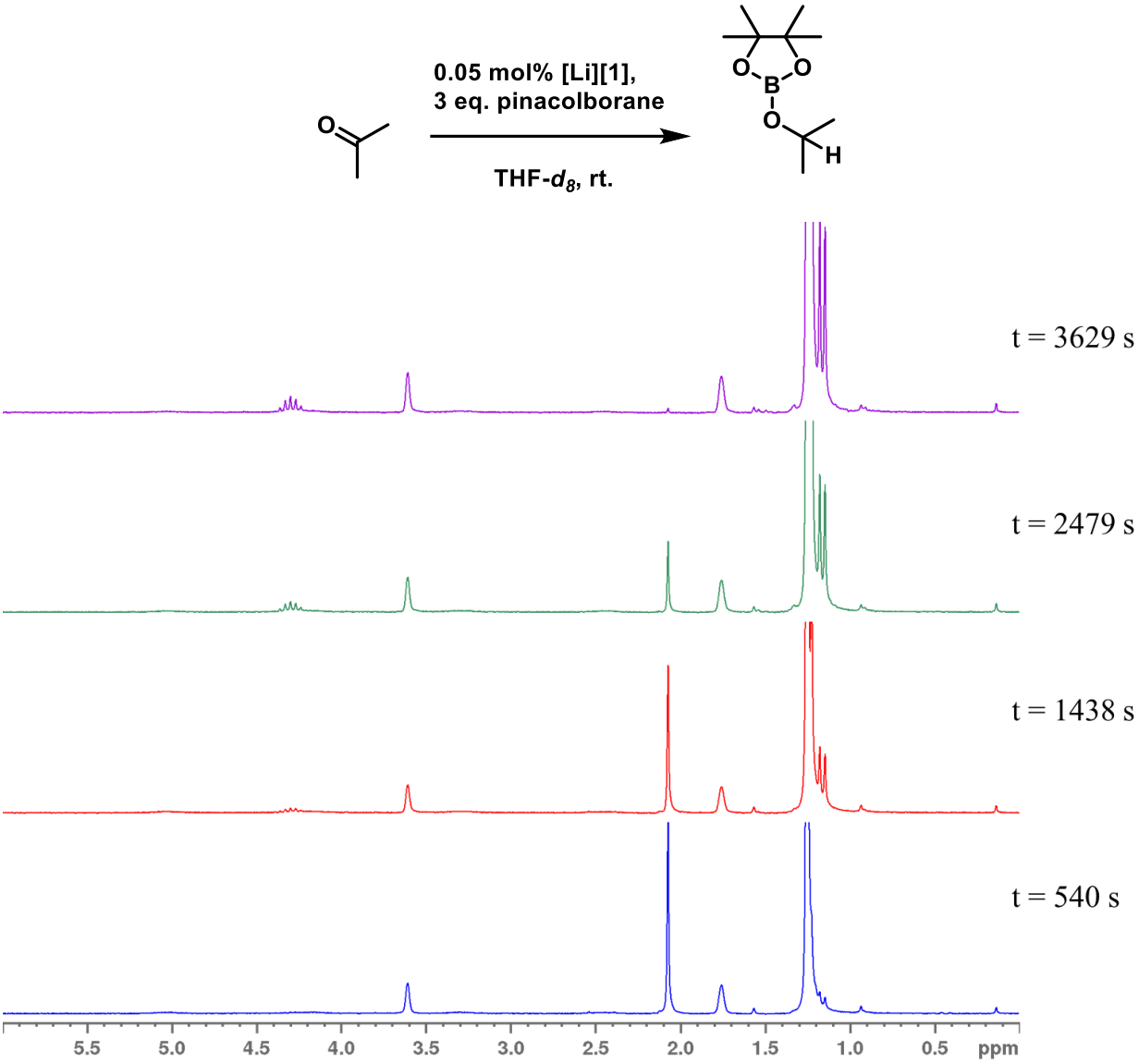


Figure S 50: Hydroboration of acetone with 0.05 mol% [Li][**1**] followed over time by ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K).

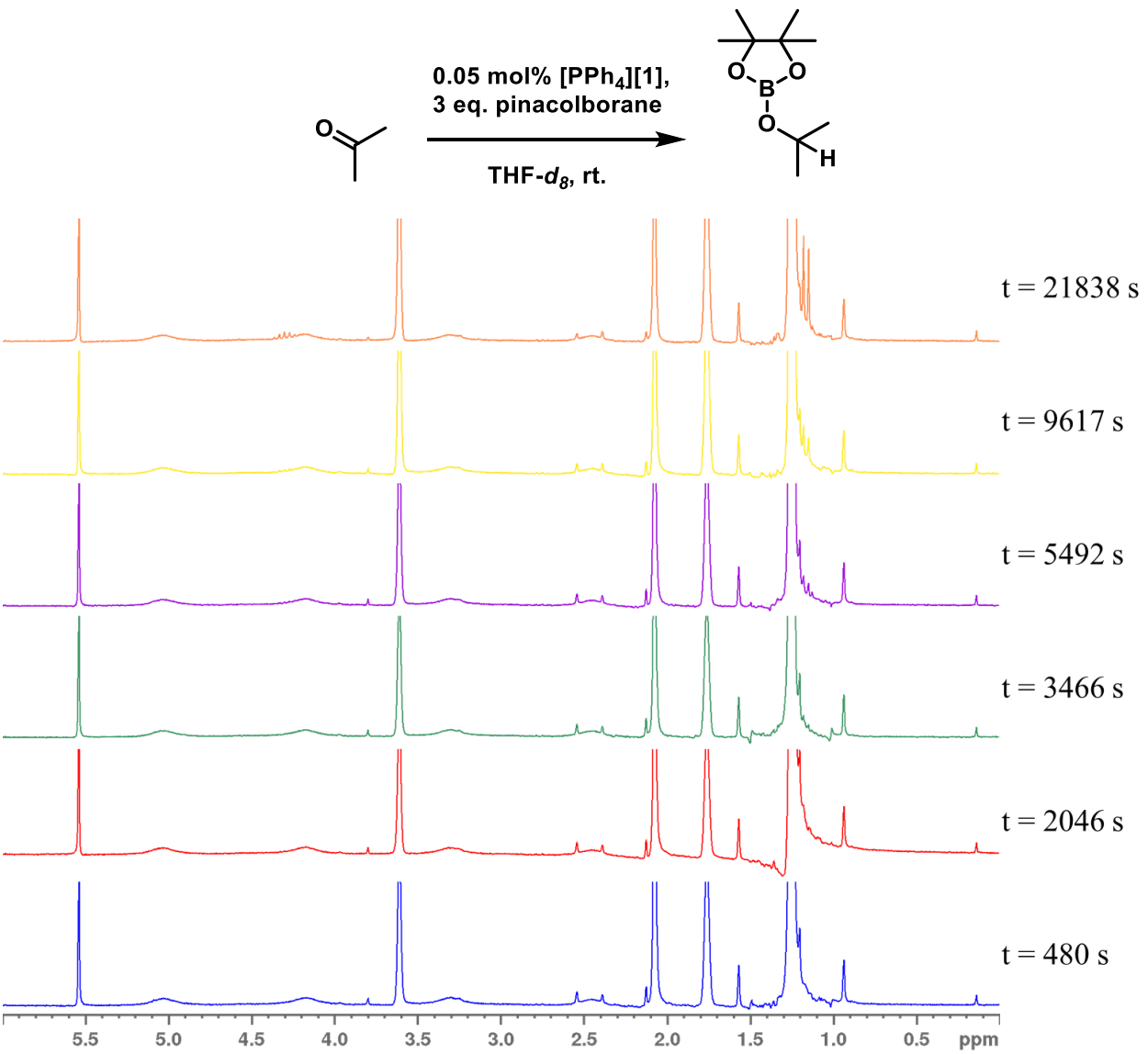


Figure S 51: Hydroboration of acetone with 0.05 mol% [PPh_4][**1**] followed over time by ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K).

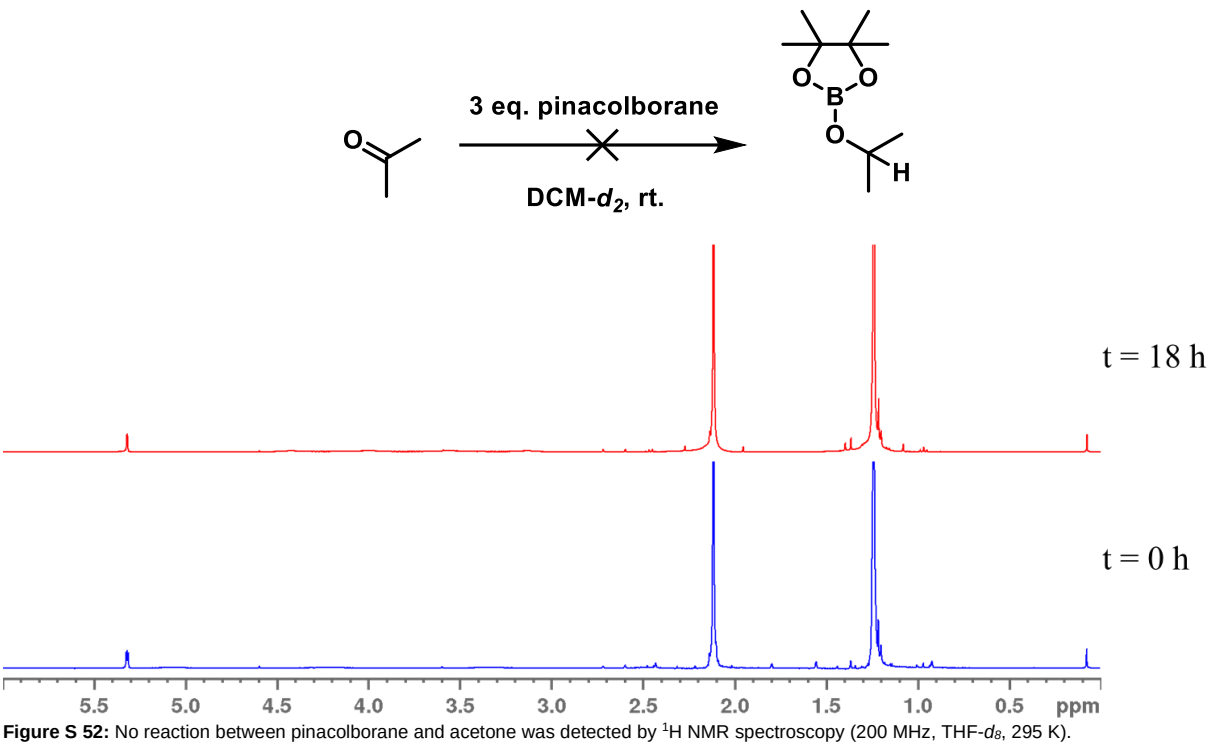


Figure S 52: No reaction between pinacolborane and acetone was detected by ^{1}H NMR spectroscopy (200 MHz, THF-d_8, 295 K).

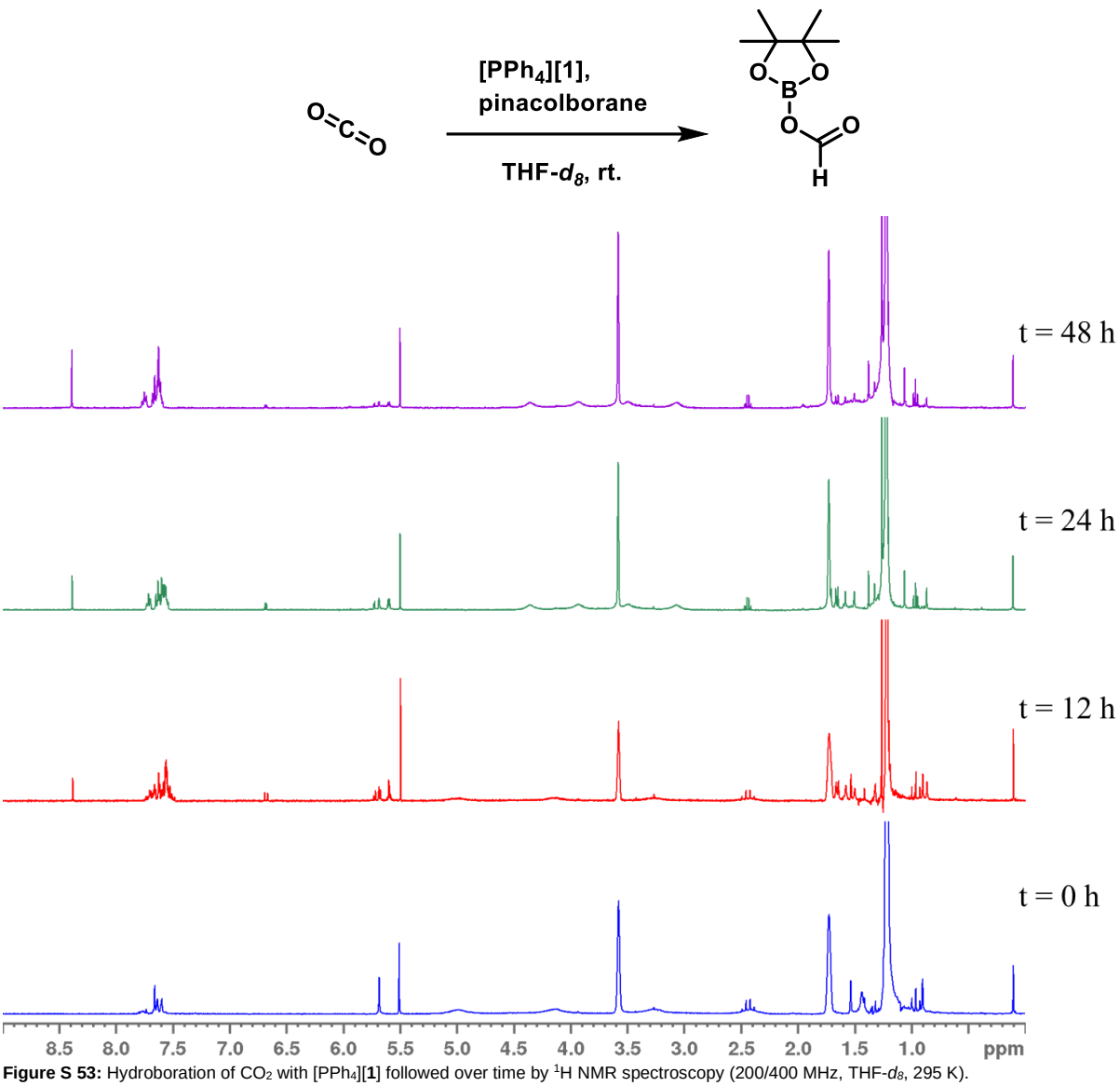


Figure S 53: Hydroboration of CO_2 with [PPh_4][**1**] followed over time by ^1H NMR spectroscopy (200/400 MHz, THF-d_8, 295 K).

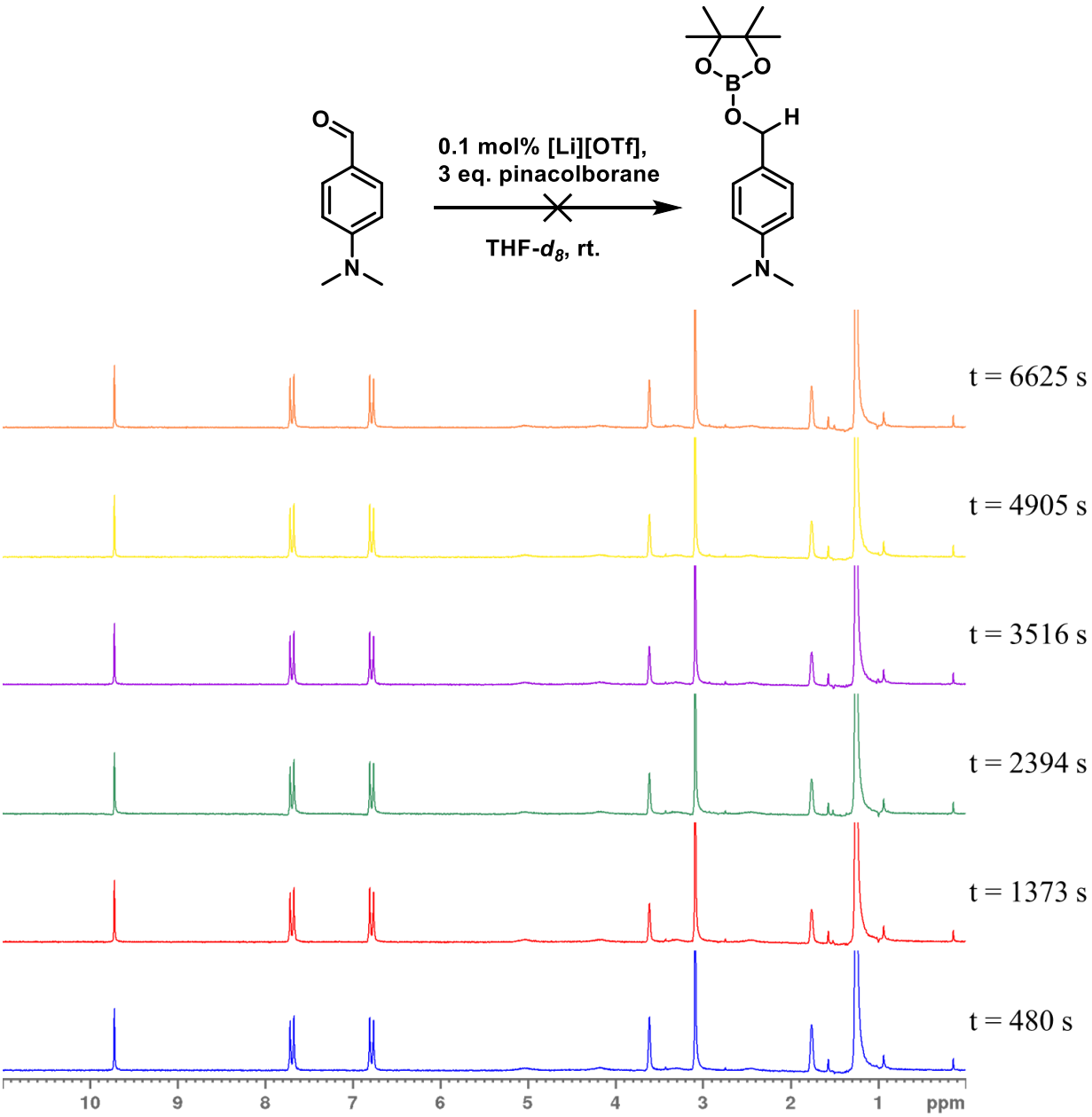


Figure S 54: No reaction between *p*DMA-BA and pinacolborane was detected with 0.1mol% [Li][OTf] by ^{1}H NMR spectroscopy(200 MHz, THF-d_8, 295 K).

10. **X-ray diffraction structures**

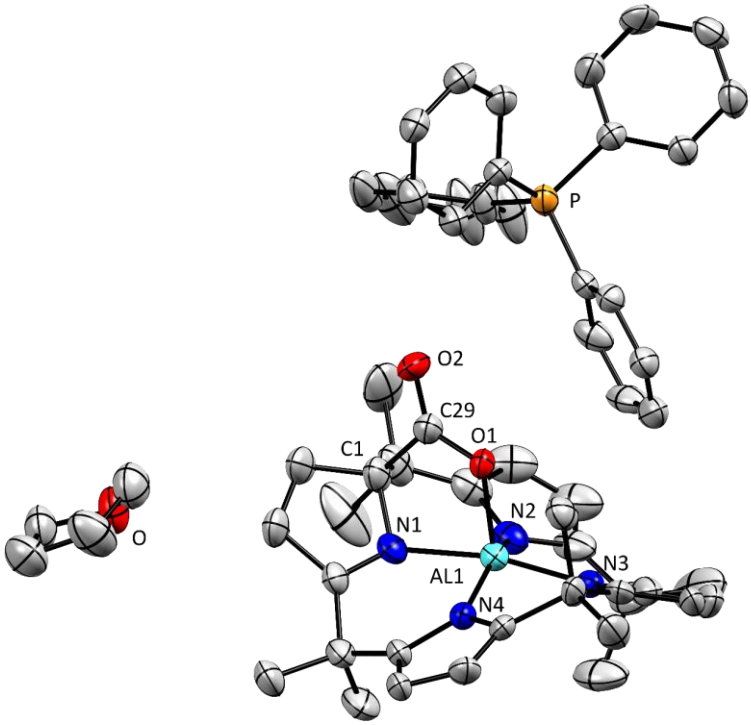


Figure S55. Molecular structure of $[PPh_4][\mathbf{1}^*\text{-}CO_2]$. Hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn with a probability of 50 %. Selected bond distances (pm): Al-O(1) 185.0(3), Al- Al-N(1) 197.0(3), N(2) 192.1(4), Al-N(3) 189.6(3), Al-N(4) 192.9(3), O(1)-C(29) 129.9(4), O(2)-C(29) 121.7(4), C(1)-C(29) 156.0(5). Selected bond angles (deg): N(1)-Al-N(3) 168.56(14), N(2)-Al-N(4)152.83(15), O(2)-C(29)-O(1) 126.3(4).

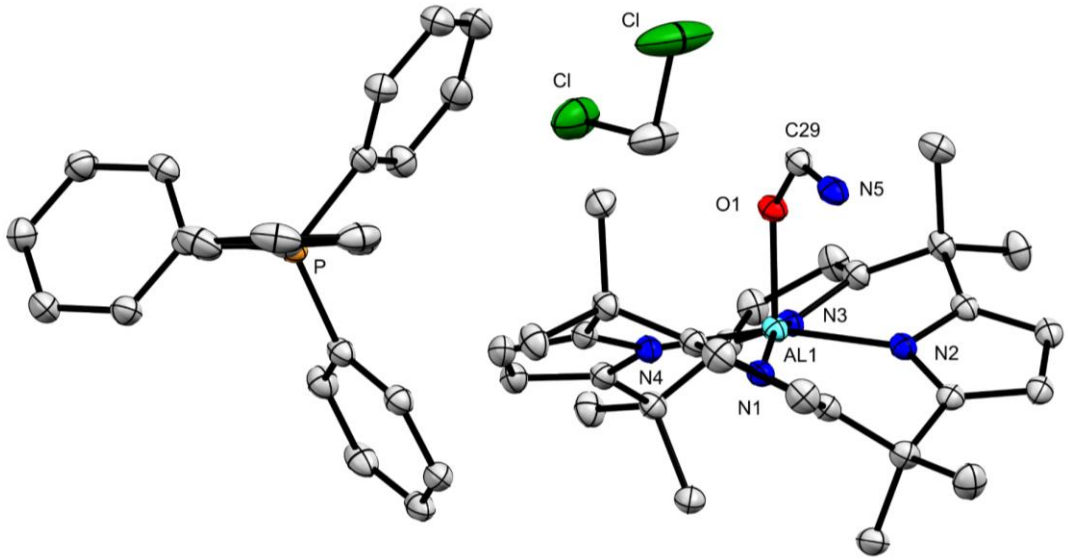


Figure S56. Molecular structure of $[PPh_4][\mathbf{1}\text{-formanide}]$. Hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn with a probability of 50 %. Selected bond distances (pm): Al(1)-O(1) 185.6(3), Al(1)-N(1) 193.8(3), Al(1)-N(2) 195.7(3), Al(1)-N(3) 194.1(3), Al(1)-N(4) 194.9(3), O(1)-C(29) 126.1(3), C(29)-N(5) 129.5(3). Selected bond angles (deg): N(1)-Al(1)-N(3) 162.52(7), N(4)-Al(1)-N(2) 163.08(7), O(1)-C(29)-N(5) 126.68(18).

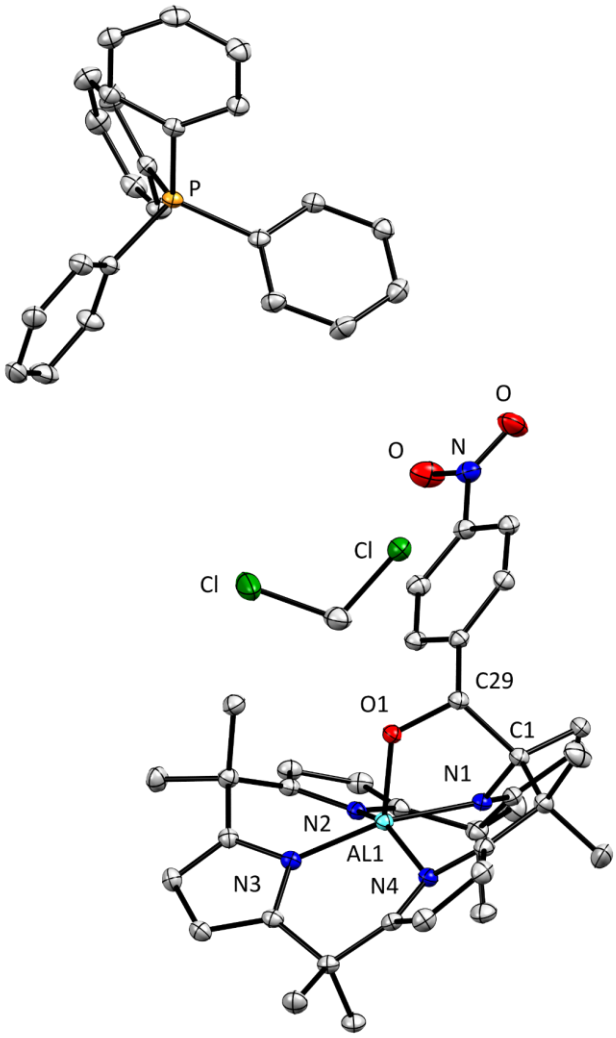


Figure S57. Molecular structure of $[PPh_4]$[**1***-*p*-nitrobenzaldehyde]. Hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn with a probability of 50 %. Selected bond distances (pm): Al(1)-O(1) 179.96(11), Al(1)-N(1) 199.08(13), Al(1)-N(2) 195.24(13), Al(1)-N(3) 191.79(13), Al(1)-N(4) 193.50(13), O(1)-C(29) 139.62(17), C(1)-C(29) 160.1(2). Selected bond angles (deg): N(1)-Al(1)-N(3) 149.42(6), N(2)-Al(1)-N(4) 165.51(6).

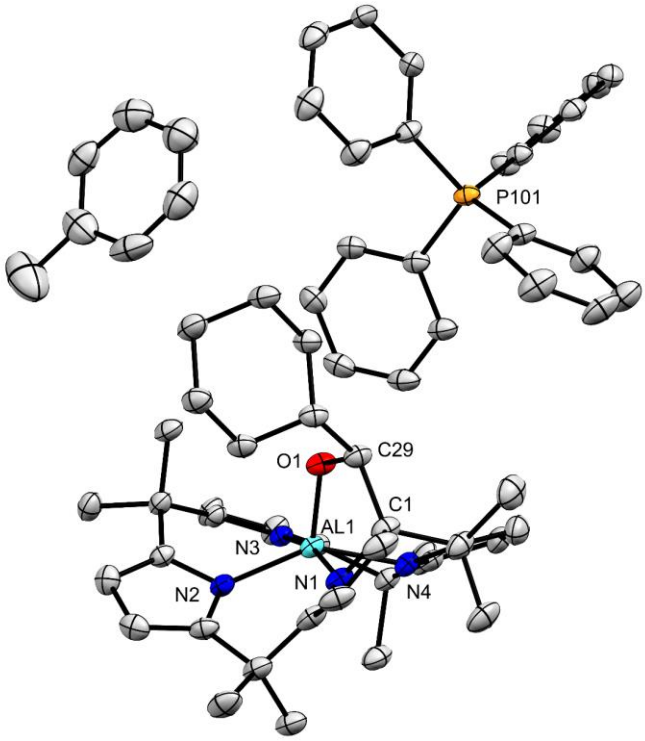


Figure S58. Molecular structure of [PPh_4][**1***-cyclohexanecarboxaldehyde]. Hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn with a probability of 50 %. Selected bond distances (pm): Al(1)-O(1) 176.73(17), Al(1)-N(1) 191.03(19), Al(1)-N(2) 194.7(2), Al(1)-N(3) 195.4(2), Al(1)-N(4) 198.4(2), O(1)-C(29) 139.8(3), C(1)-C(29) 159.9(3). Selected bond angles (deg): N(1)-Al(1)-N(3) 167.67(8), N(4)-Al(1)-N(2) 147.34(8).

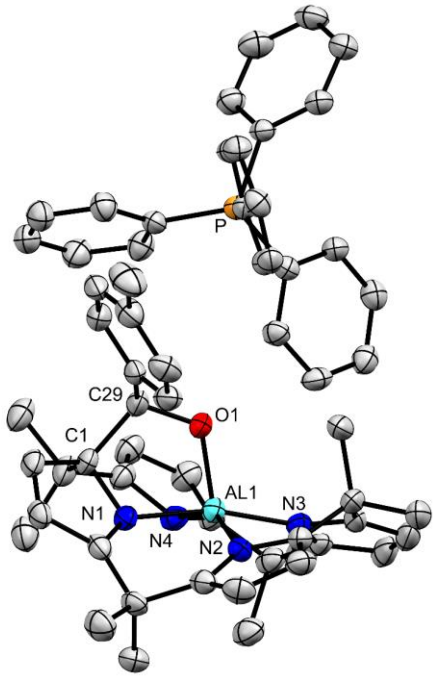


Figure S59. Molecular structure of [PPh_4][**1***-*p*-methylbenzaldehyde]. Hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn with a probability of 50 %. Selected bond distances (pm): Al(1)-O(1) 179.0(2), Al(1)-N(1) 197.2(3), Al(1)-N(2) 196.1(2), Al(1)-N(3) 191.5(3), Al(1)-N(4) 195.5(2), O(1)-C(29) 141.0(3), C(1)-C(29) 159.6(4). Selected bond angles (deg): N(1)-Al(1)-N(3) 166.05(11), N(4)-Al(1)-N(2) 149.89(11).

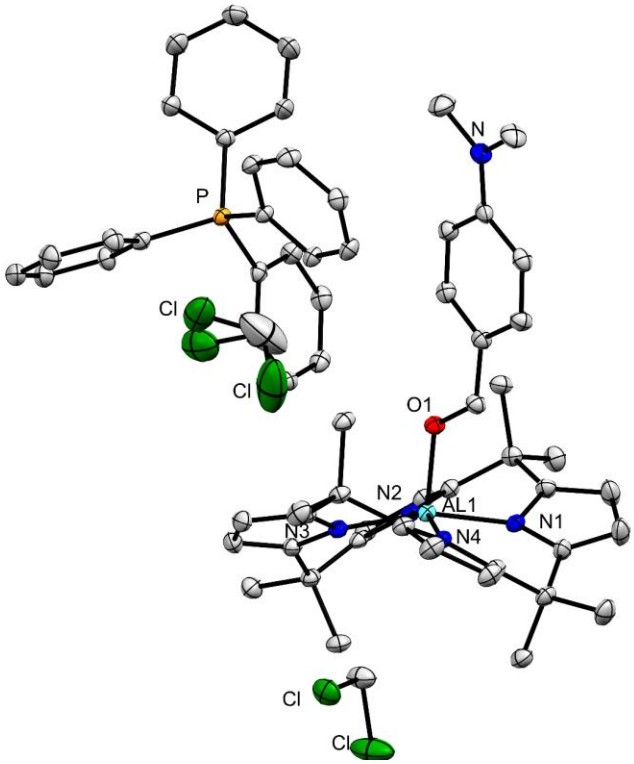


Figure S60. Molecular structure of [PPh_4][**1**-*p*-dimethylaminobenzaldehyde]. Hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn with a probability of 50 %. Selected bond distances (pm): Al(1)-O(1) 189.8(2), Al(1)-N(1) 194.1(2), Al(1)-N(2) 194.4(2), Al(1)-N(3) 194.7(2), Al(1)-N(4) 194.4(2), O(1)-C(29) 125.8(3). Selected bond angles (deg): N(1)-Al(1)-N(3) 163.29(10), N(4)-Al(1)-N(2) 162.84(10).

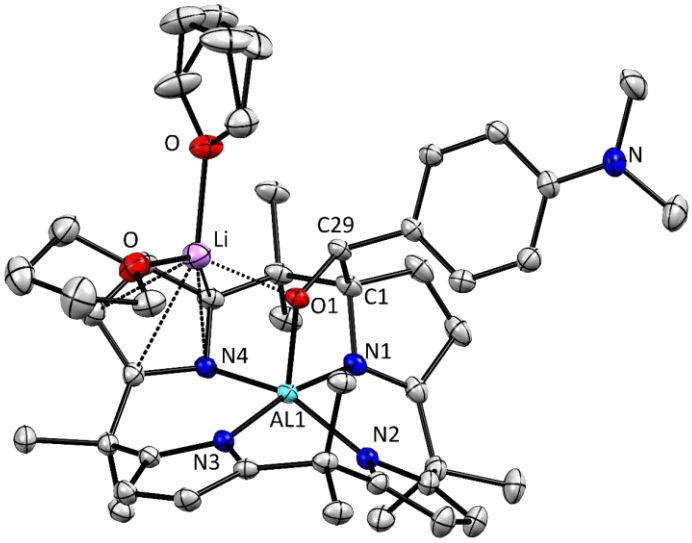


Figure S61. Molecular structure of [$Li(thf)_2$][**1***-*p*-dimethylaminobenzaldehyde]. Hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn with a probability of 50 %. Selected bond distances (pm): Al(1)-O(1) 189.8(2), Al(1)-N(1) 194.1(2), Al(1)-N(2) 194.4(2), Al(1)-N(3) 194.7(2), Al(1)-N(4) 194.4(2), O(1)-C(29) 125.8(3). Selected bond angles (deg): N(1)-Al(1)-N(3) 163.29(10), N(4)-Al(1)-N(2) 162.84(10).

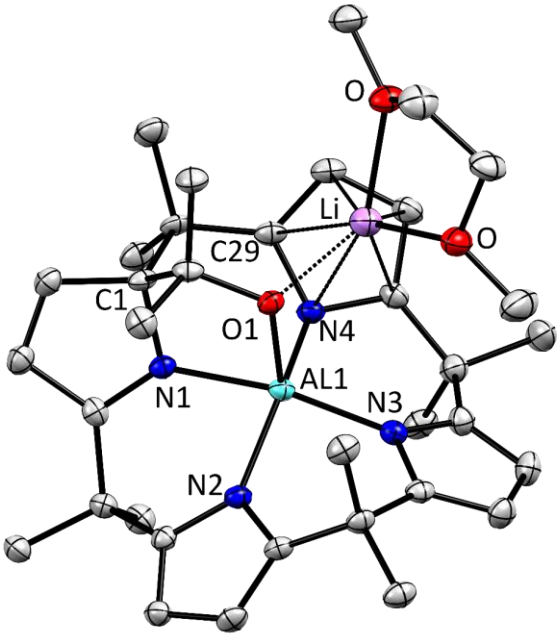


Figure S62. Molecular structure of [Li(dme)][**1***-acetone]. Hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn with a probability of 50 %. Selected bond distances (pm) and angles (deg): Al(1)-O(1) 182.2(54), Al(1)-N(1) 194.4(5), Al(1)-N(2) 198.1(5), Al(1)-N(3) 197.2(5), Al(1)-N(4) 191.2(5), O(1)-C(29) 142.3(7), C(1)-C(29) 161.0(8). Selected bond angles (deg): N(1)-Al(1)-N(3) 166.8(2), N(4)-Al(1)-N(2) 151.0(2).

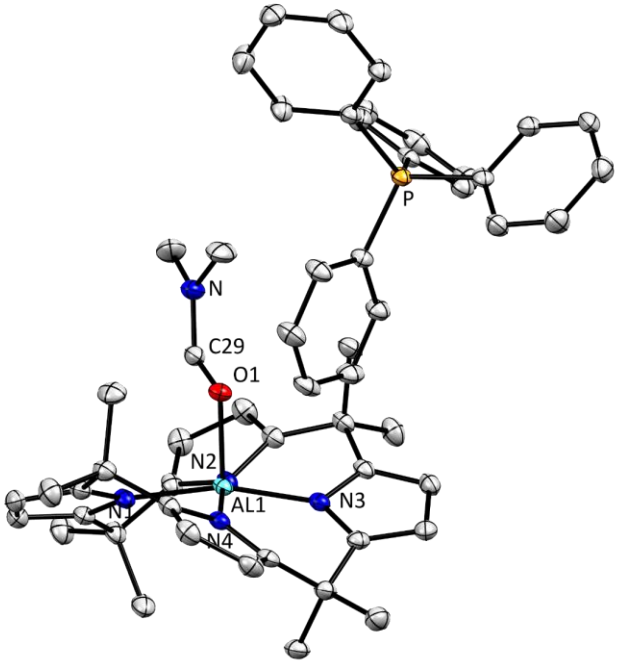


Figure S63. Molecular structure of [PPh_4][**1***-dimethylformamide]. Hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn with a probability of 50 %. Selected bond distances (pm): Al(1)-O(1) 188.43(13), Al(1)-N(1) 196.68(16), Al(1)-N(2) 195.85(16), Al(1)-N(3) 194.48(16), Al(1)-N(4) 193.04(16), O(1)-C(29) 126.4(2). Selected bond angles (deg): N(1)-Al(1)-N(3) 163.65(7), N(4)-Al(1)-N(2) 162.47(7).

11. NMR spectra of all new compounds

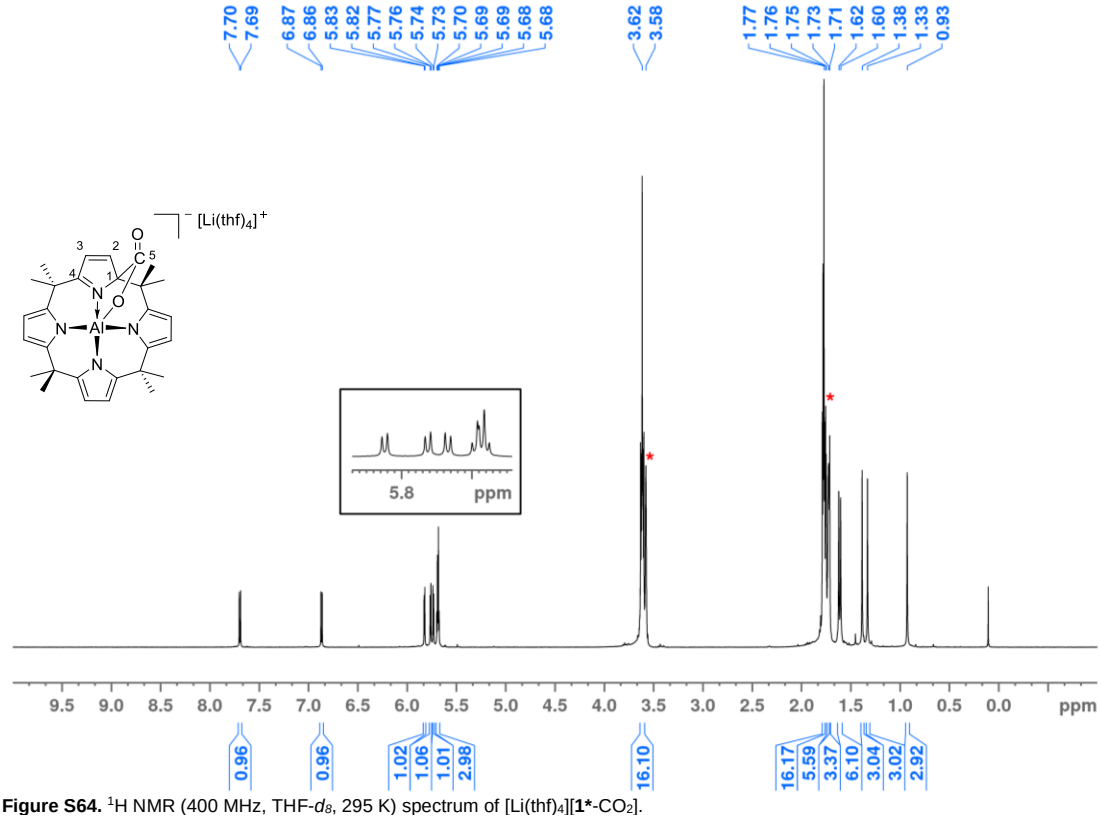


Figure S64. ^{1}H NMR (400 MHz, THF-d_8, 295 K) spectrum of [Li(thf)$_4$][**1***-CO$_2$].

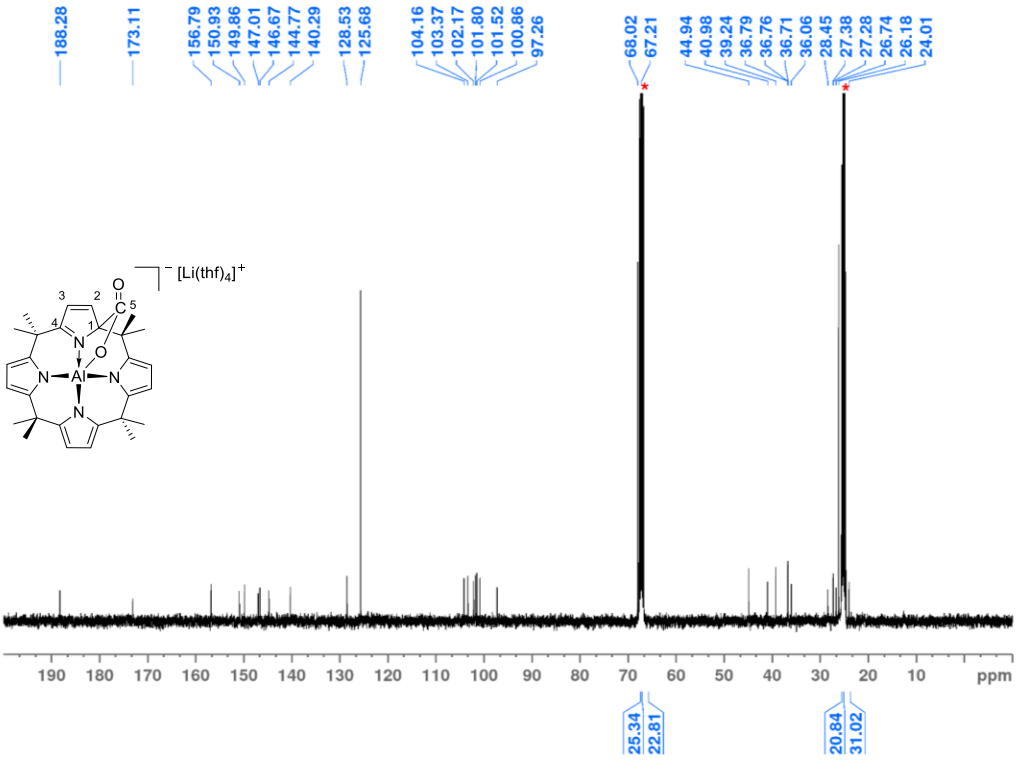


Figure S65. ^{13}C{^{1}H} NMR (100 MHz, DCM-d_2, 295 K) spectrum of [Li(thf)$_4$][**1***-CO$_2$].

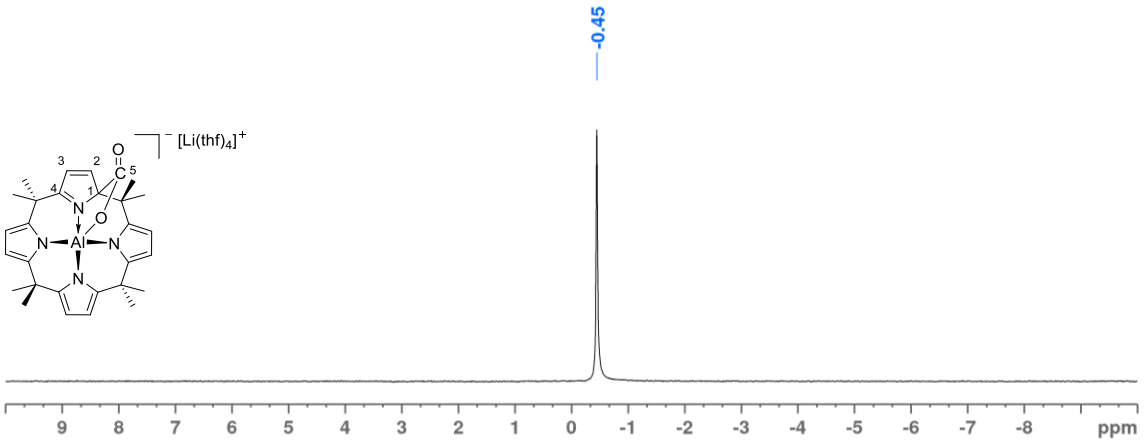


Figure S66. ^{7}Li NMR (155 MHz, THF-d_8, 295 K) spectrum of [Li(thf)$_4$][**1***-CO$_2$].

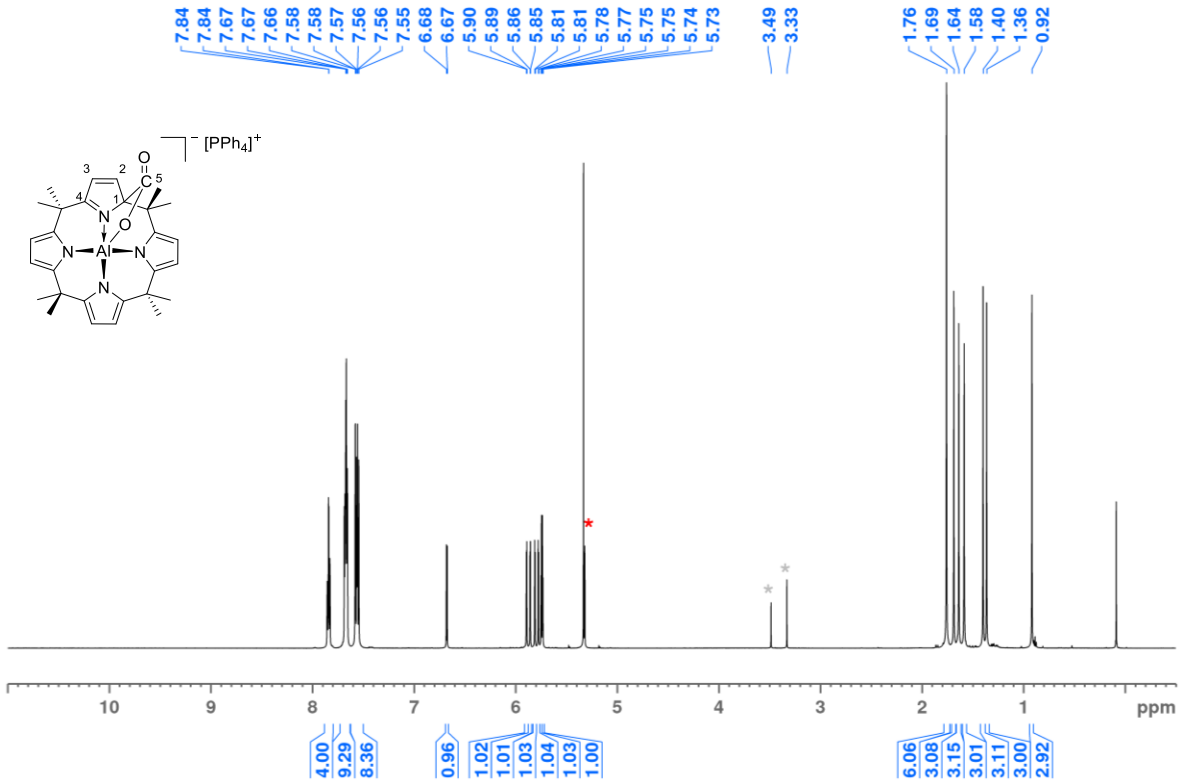


Figure S 67: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectrum of [PPh$_4$][**1***-CO$_2$]. The gray asterisk marks residual dimethoxyethane.

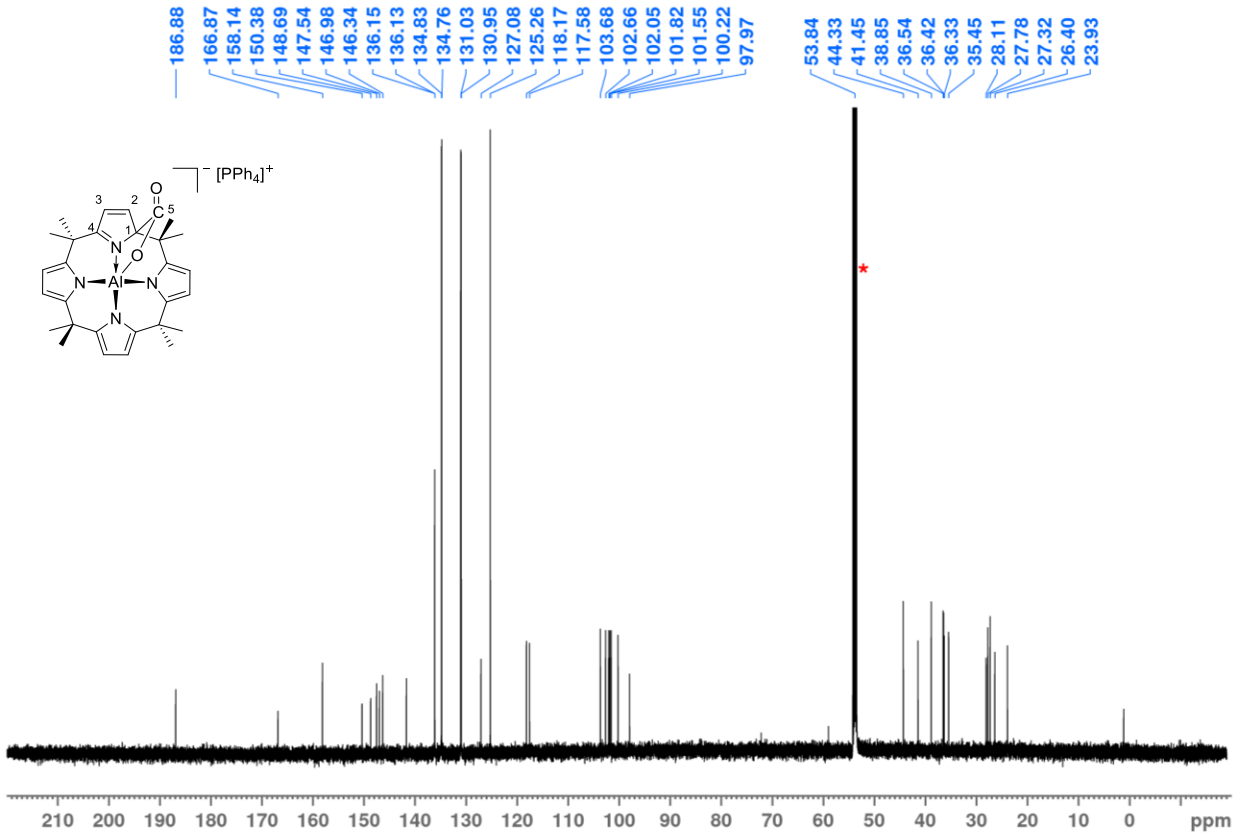


Figure S 68: $^{13}C\{^{1}H\}$ NMR (150 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1***-CO_2].

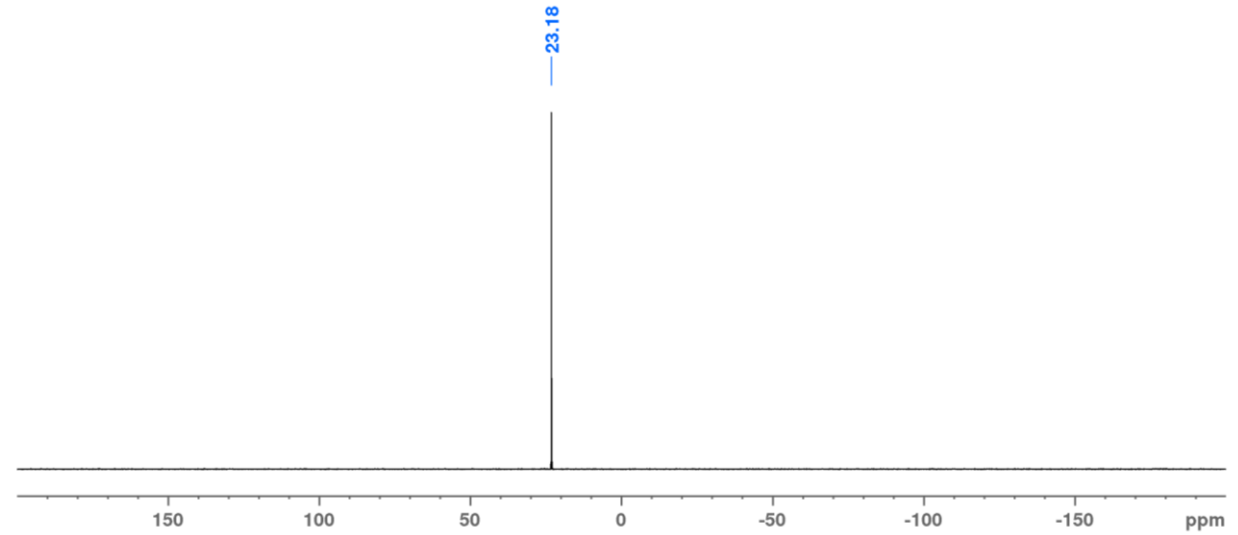


Figure S 69: ^{31}P NMR (243 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1***-CO_2].

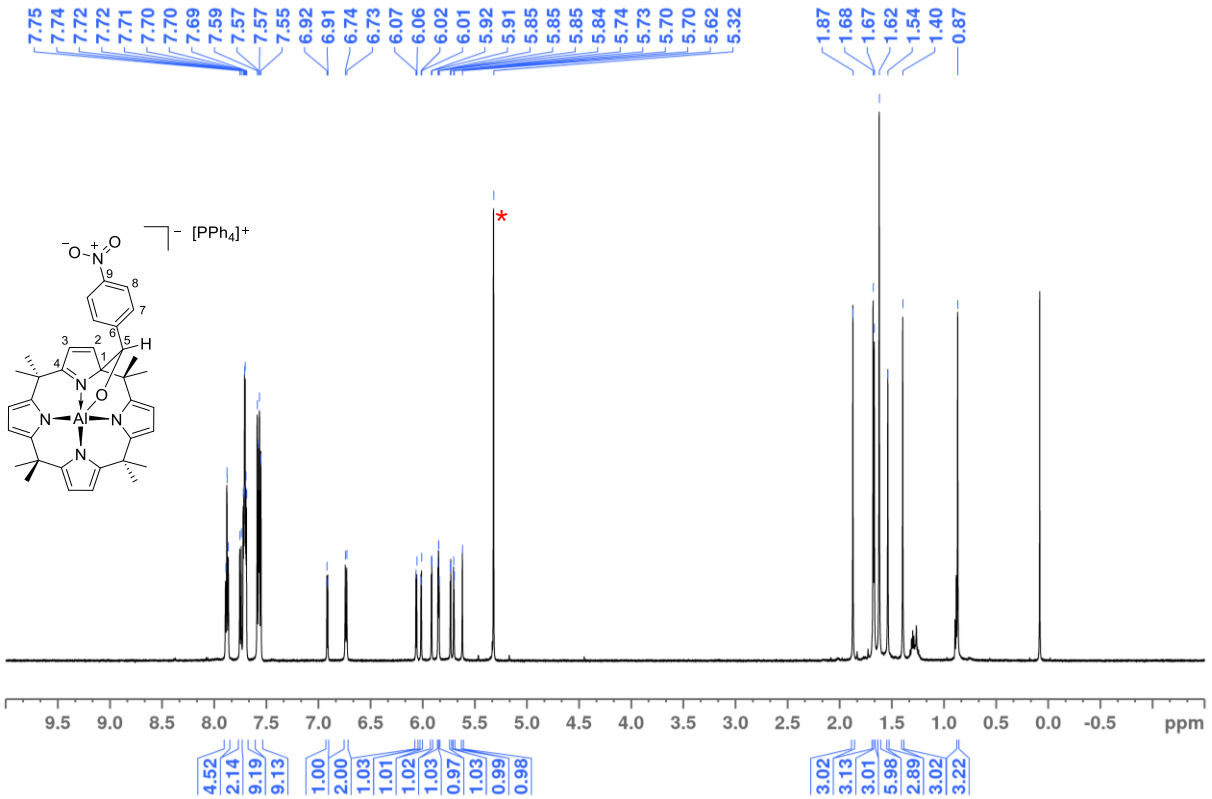


Figure S 70: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectrum of [PPh$_4$][**1***-*p*-nitrobenzaldehyde].

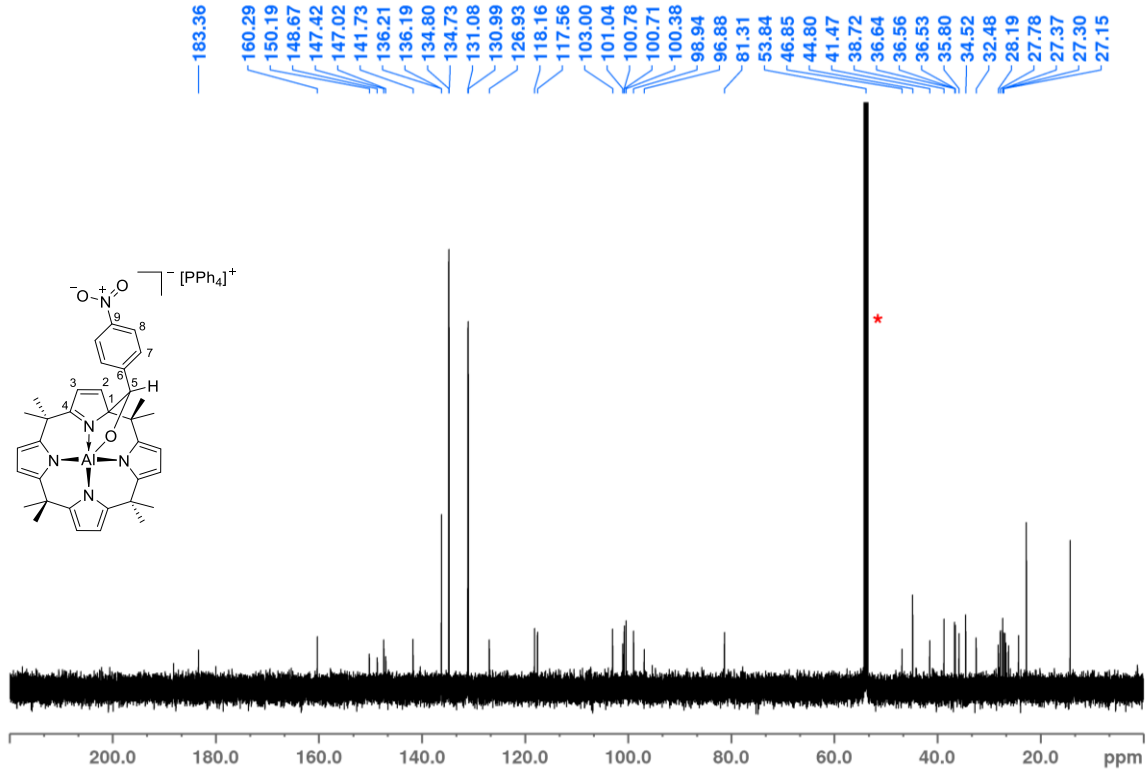


Figure S 71: ^{13}C{^{1}H} NMR (150 MHz, DCM-d_2, 295 K) spectrum of [PPh$_4$][**1***-*p*-nitrobenzaldehyde].

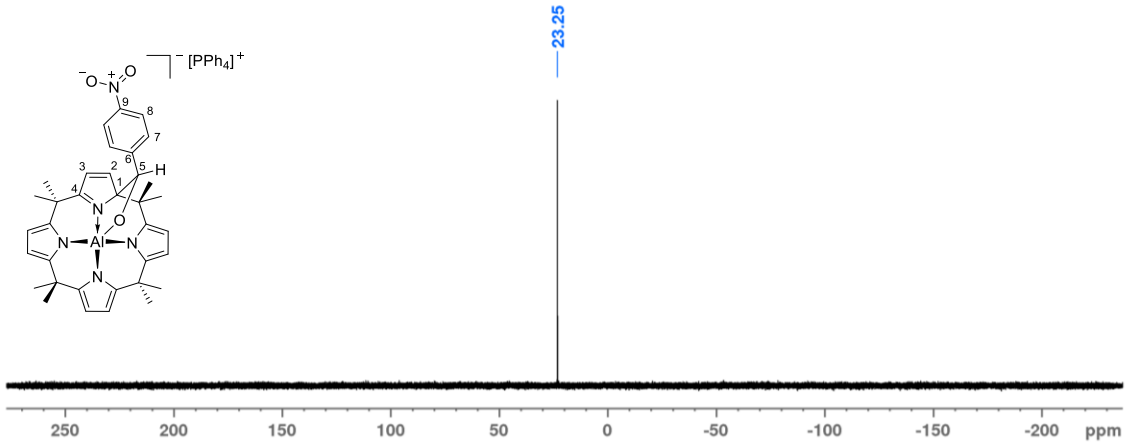


Figure S 72: ^{31}P NMR (243 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1***- *p*-nitrobenzaldehyde].

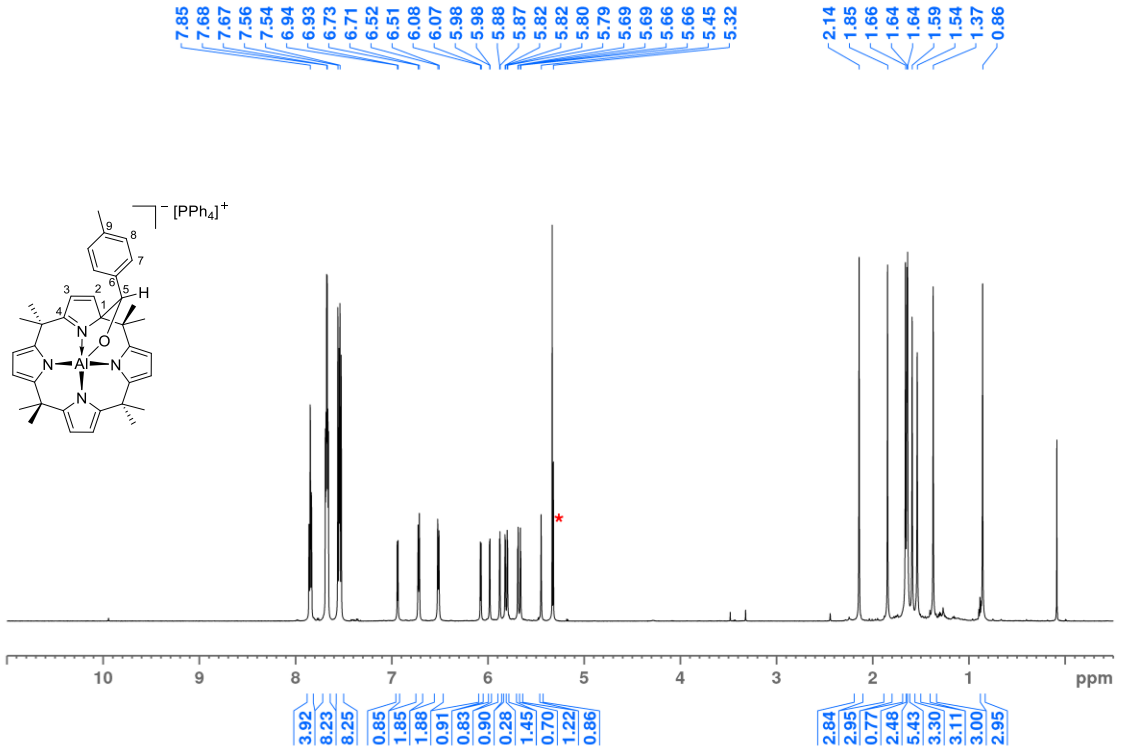


Figure S 73: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1***-*p*-methylbenzaldehyde].

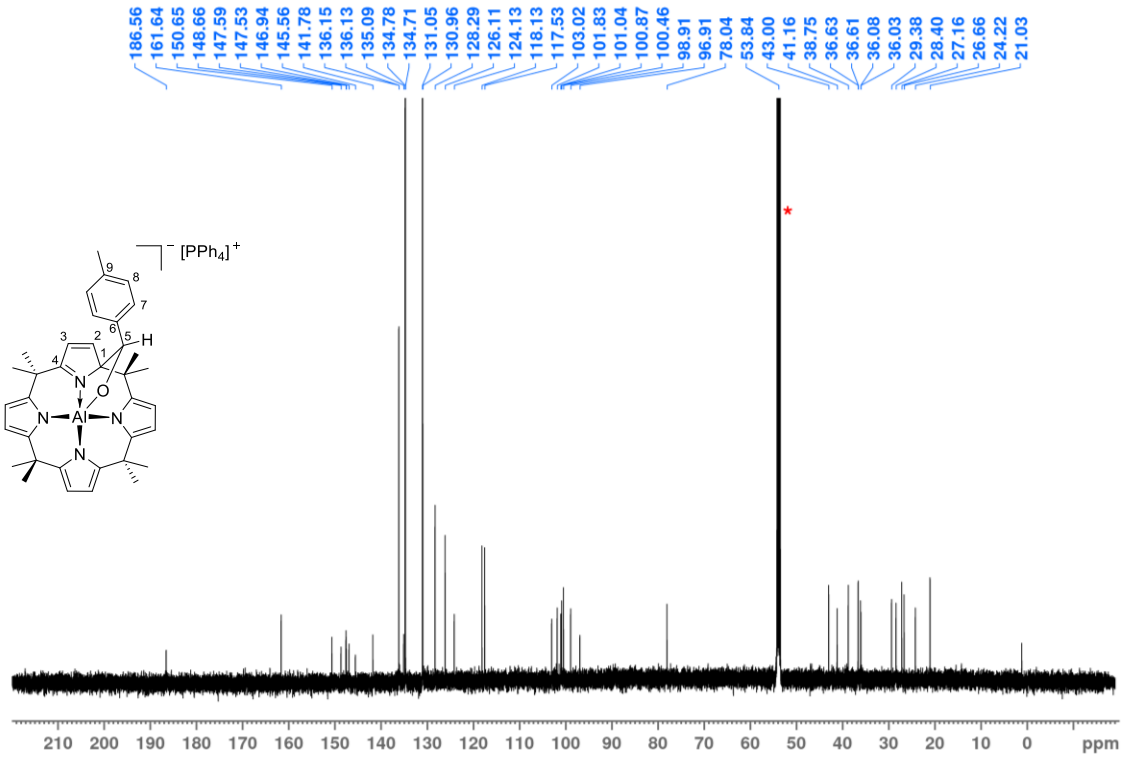


Figure S 74: $^{13}C\{^{1}H\}$ NMR (150 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1***-*p*-methylbenzaldehyde].

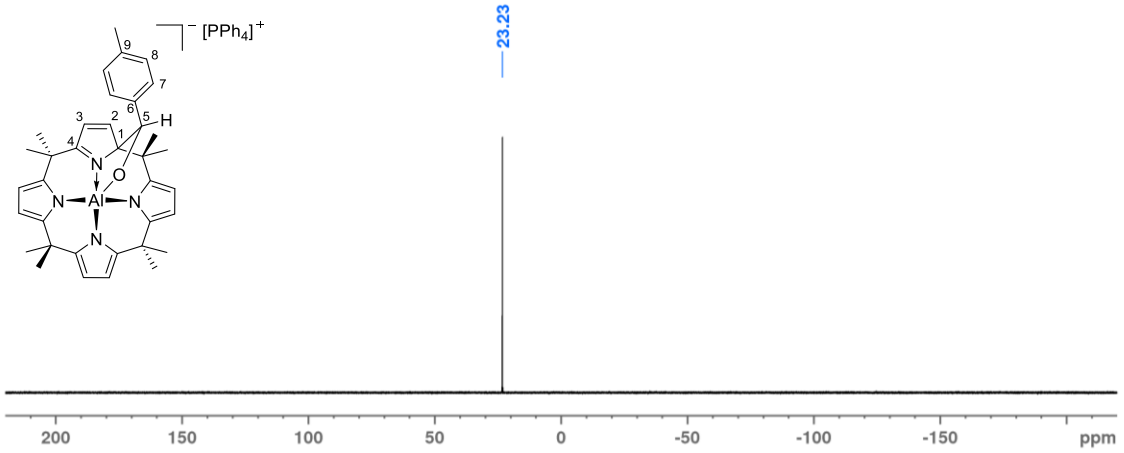


Figure S 75: ^{31}P NMR (162 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1***-*p*-methylbenzaldehyde].

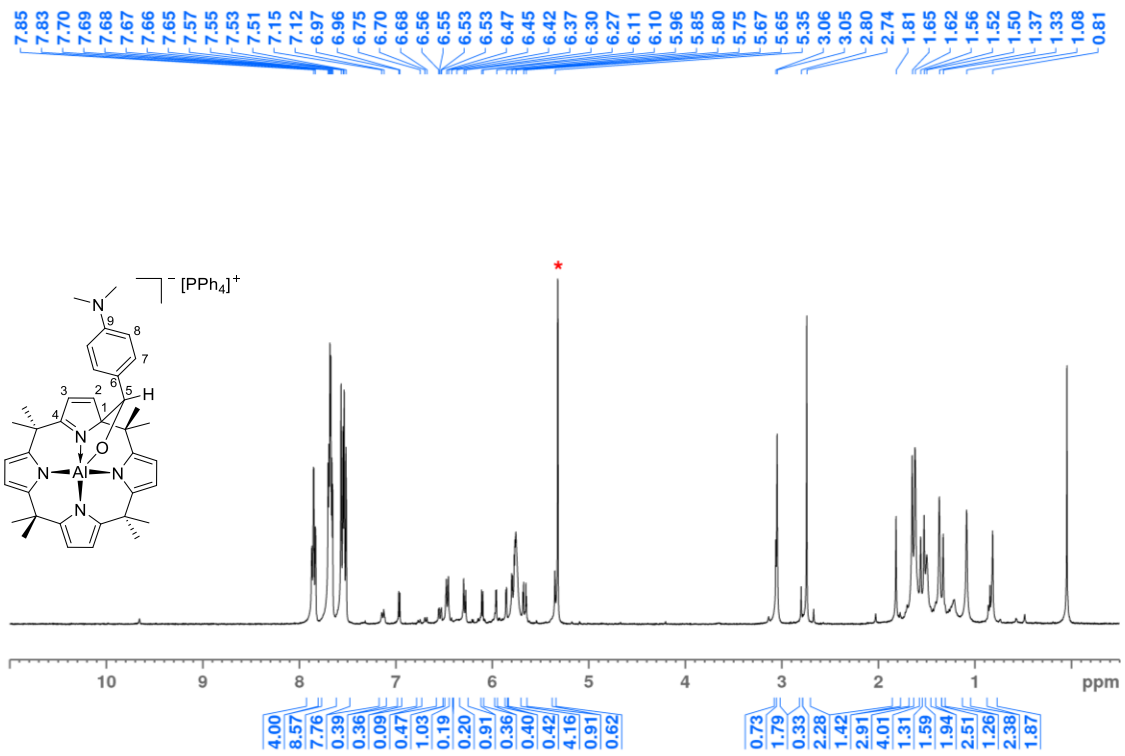


Figure S 76: ^{1}H NMR (400 MHz, DCM-d_2, 270 K) spectrum of [PPh_4][**1***-*p*-dimethylaminobenzaldehyde].

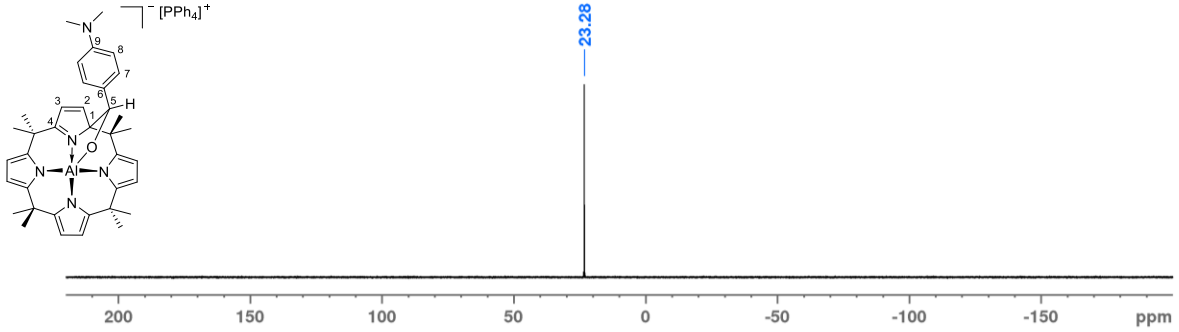


Figure S 77: ^{31}P NMR (162 MHz, DCM-d_2, 270 K) spectrum of [PPh_4][**1***-*p*-dimethylaminobenzaldehyde].

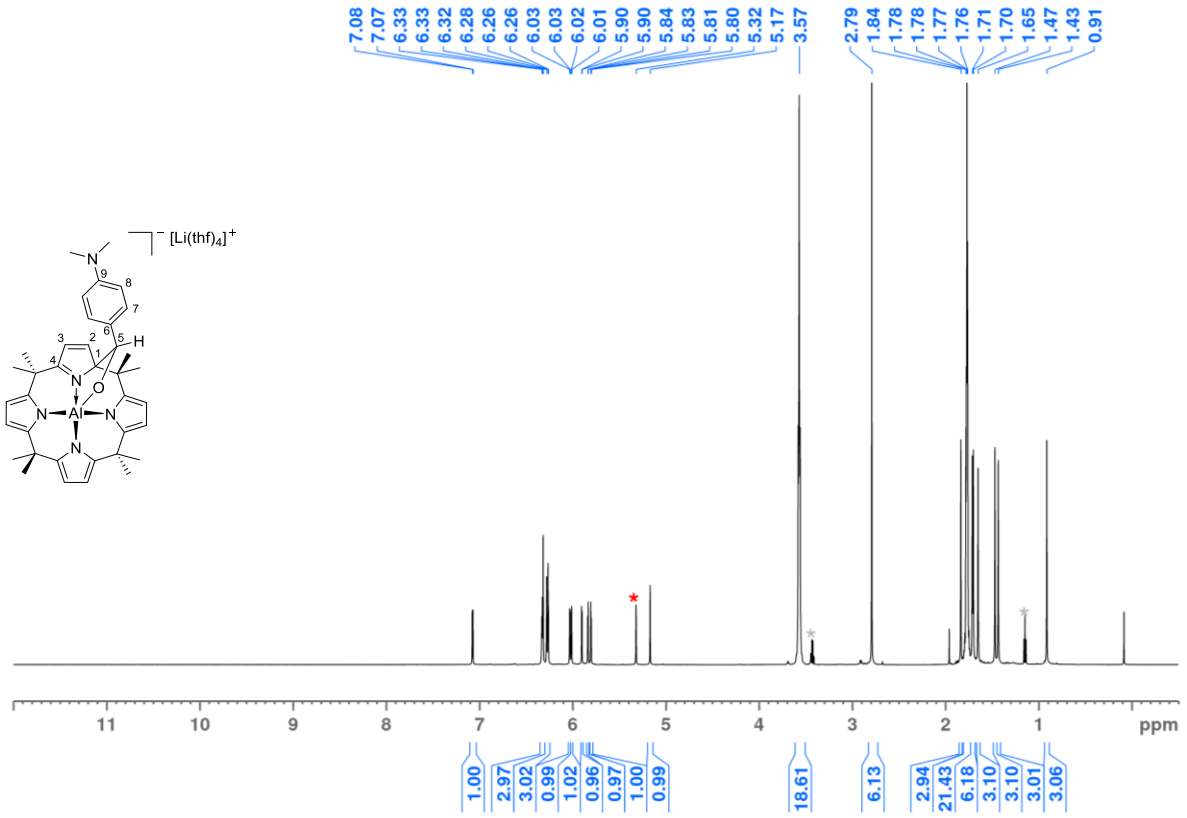


Figure S 78: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectrum of [Li(thf)$_4$][**1***-*p*-dimethylaminobenzaldehyde]. Gray asterisk marks residue of diethyl ether.

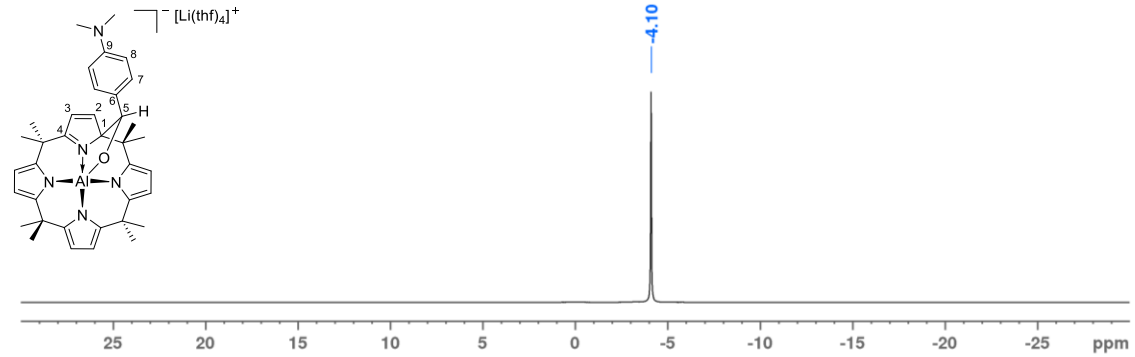


Figure S 79: ^{7}Li NMR (233 MHz, DCM-d_2, 295 K) spectrum of [Li(thf)$_4$][**1***-*p*-dimethylaminobenzaldehyde].

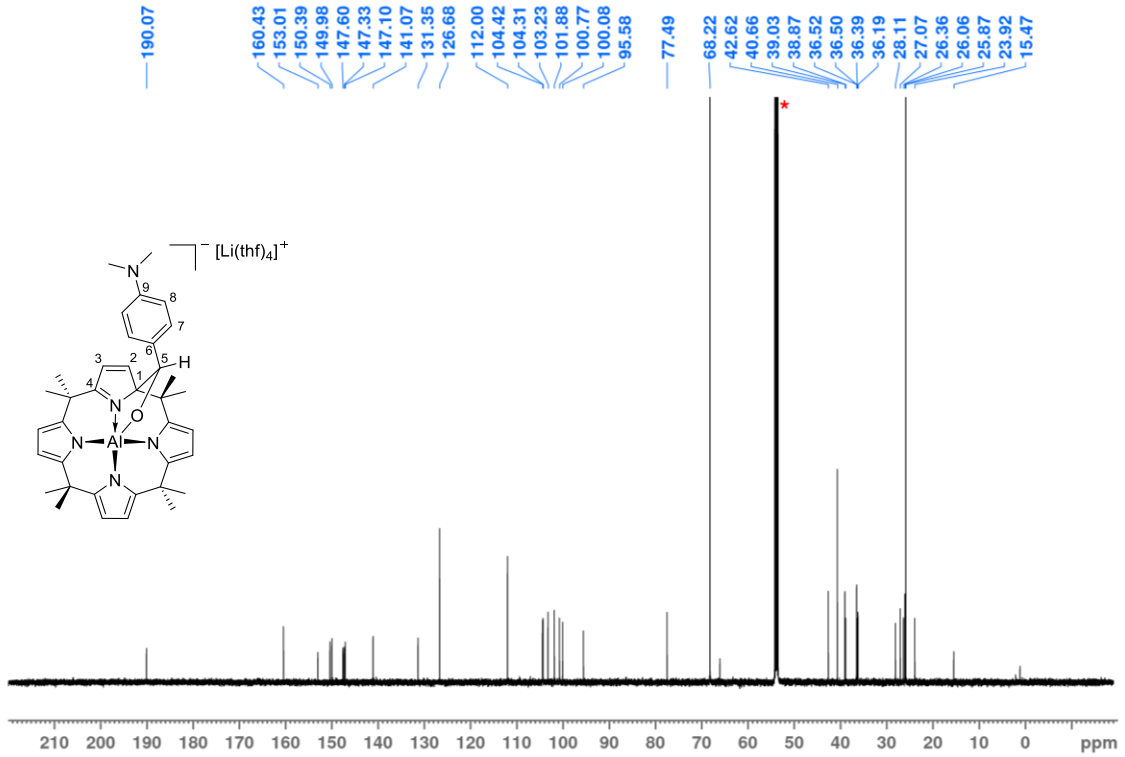


Figure S 80: $^{13}C\{^{1}H\}$ NMR (150 MHz, DCM-d_2, 295 K) spectrum of $[Li(thf)_4]$[**1***-*p*-dimethylaminobenzaldehyde].

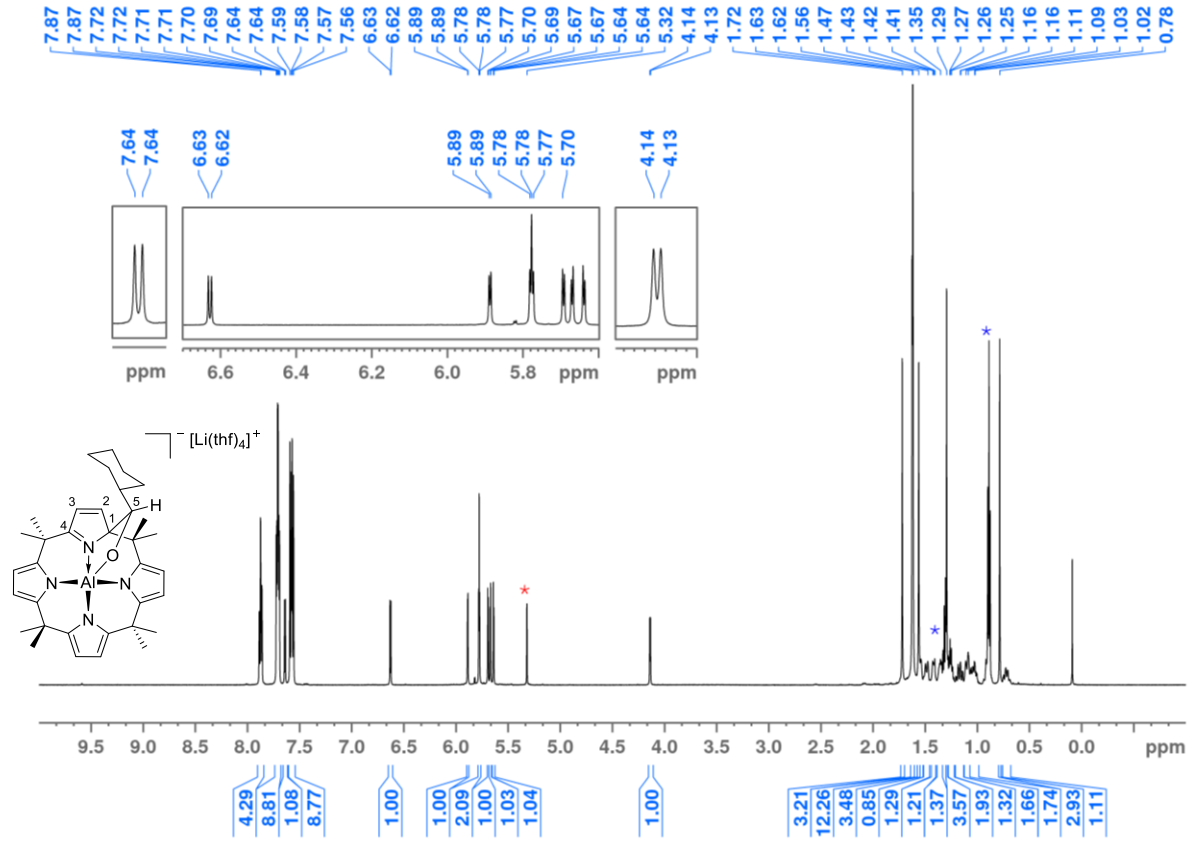


Figure S 81: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectrum of $[PPh_4]$[**1***-cyclohexanecarboxaldehyde]. Purple asterisks mark residues of *n*-pentane.

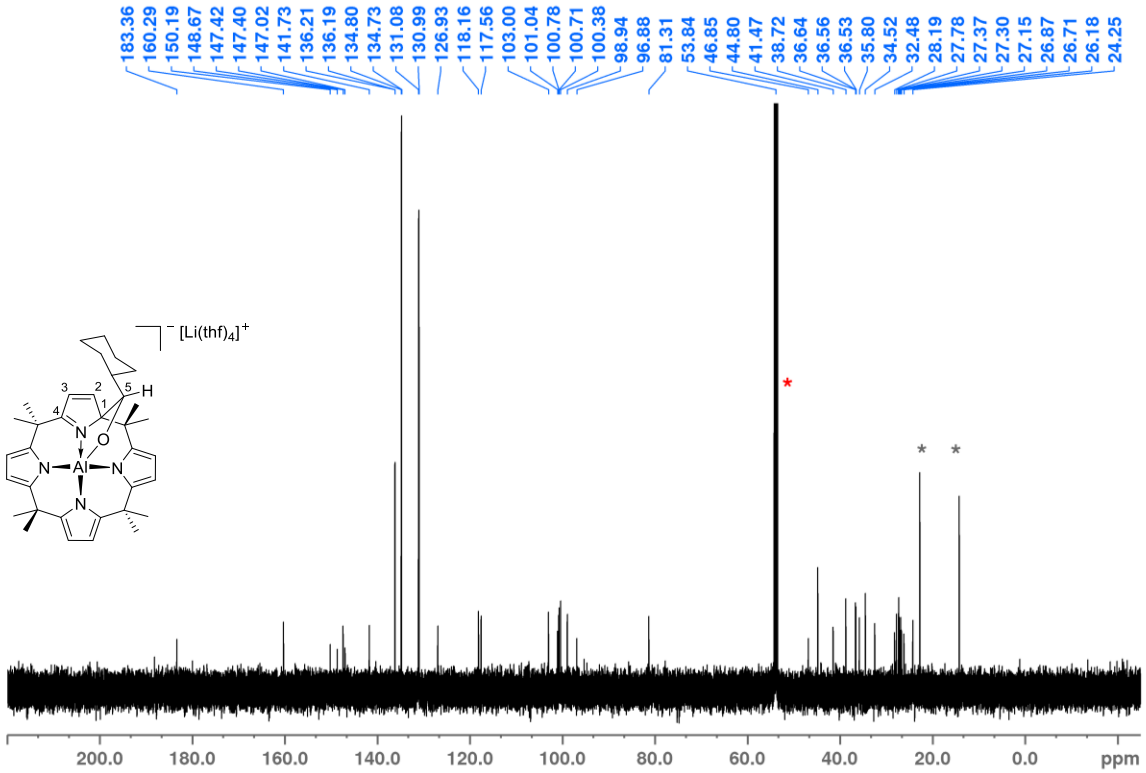


Figure S 82: $^{13}C\{^{1}H\}$ NMR (150 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1***-cyclohexanecarboxaldehyde]. Gray asterisks mark residues of *n*-pentane.

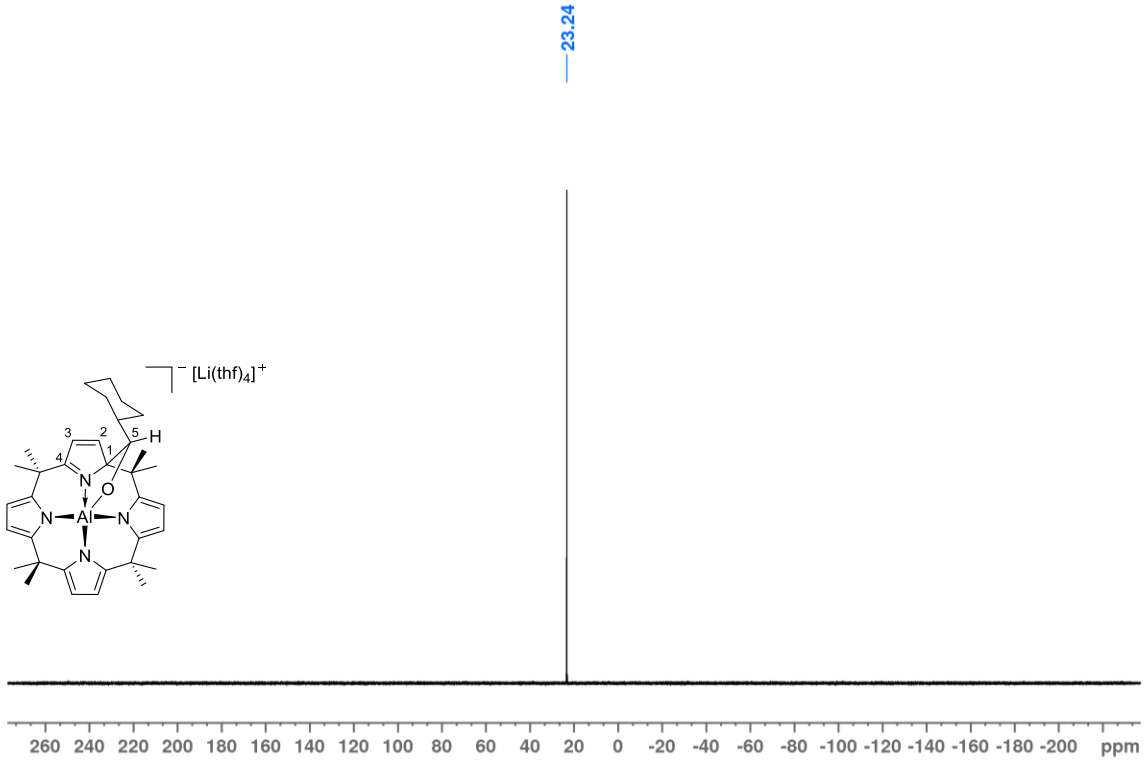


Figure S 83: ^{31}P NMR (243 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1***-cyclohexanecarboxaldehyde].

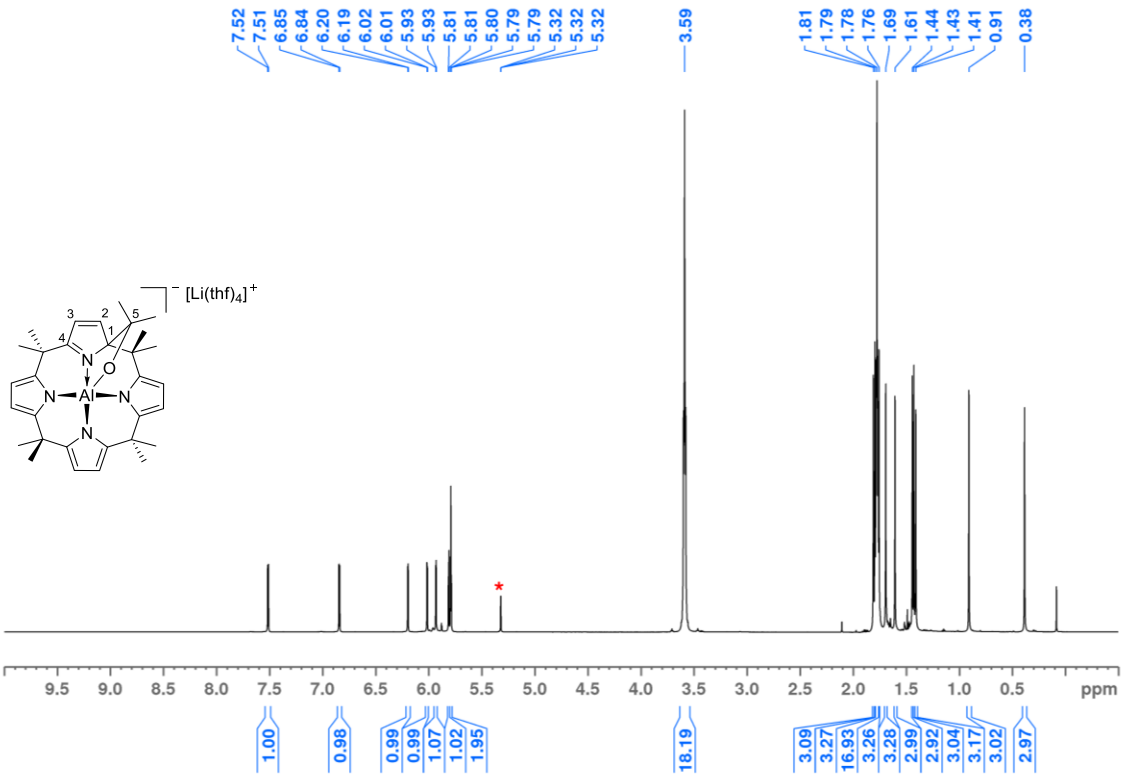


Figure S 84: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectrum of [Li(thf)$_4$][**1***-acetone].

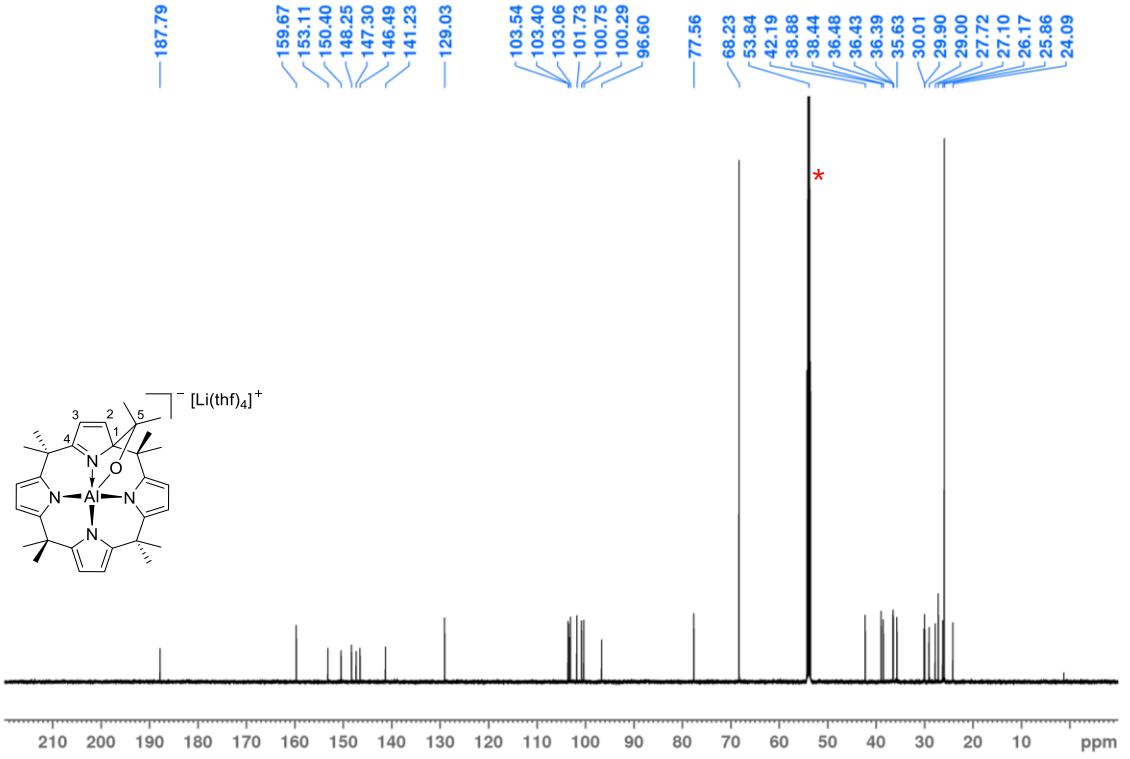


Figure S 85: ^{13}C{^{1}H} NMR (150 MHz, DCM-d_2, 295 K) spectrum of [Li(thf)$_4$][**1***-acetone].

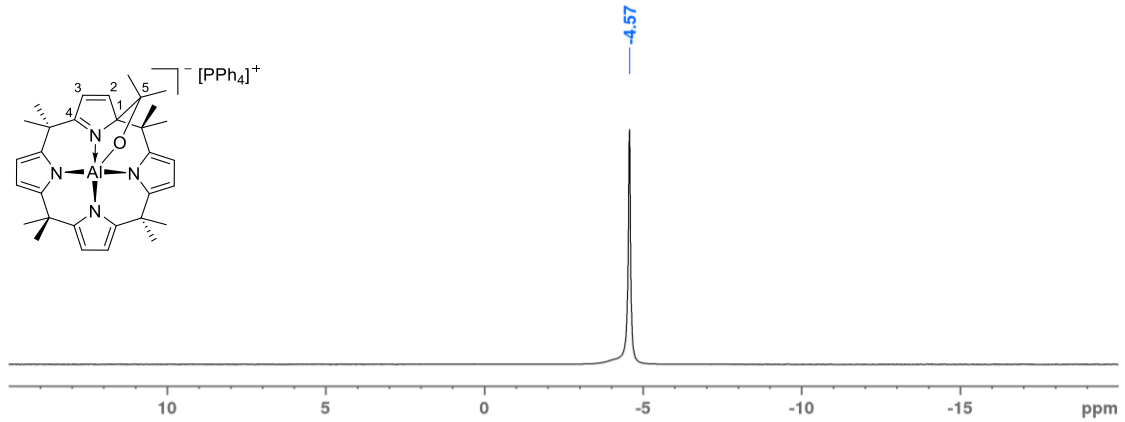


Figure S 86: ^{7}Li NMR (233 MHz, DCM-d_2, 295 K) spectrum of [Li(thf)$_4$][**1***-acetone].

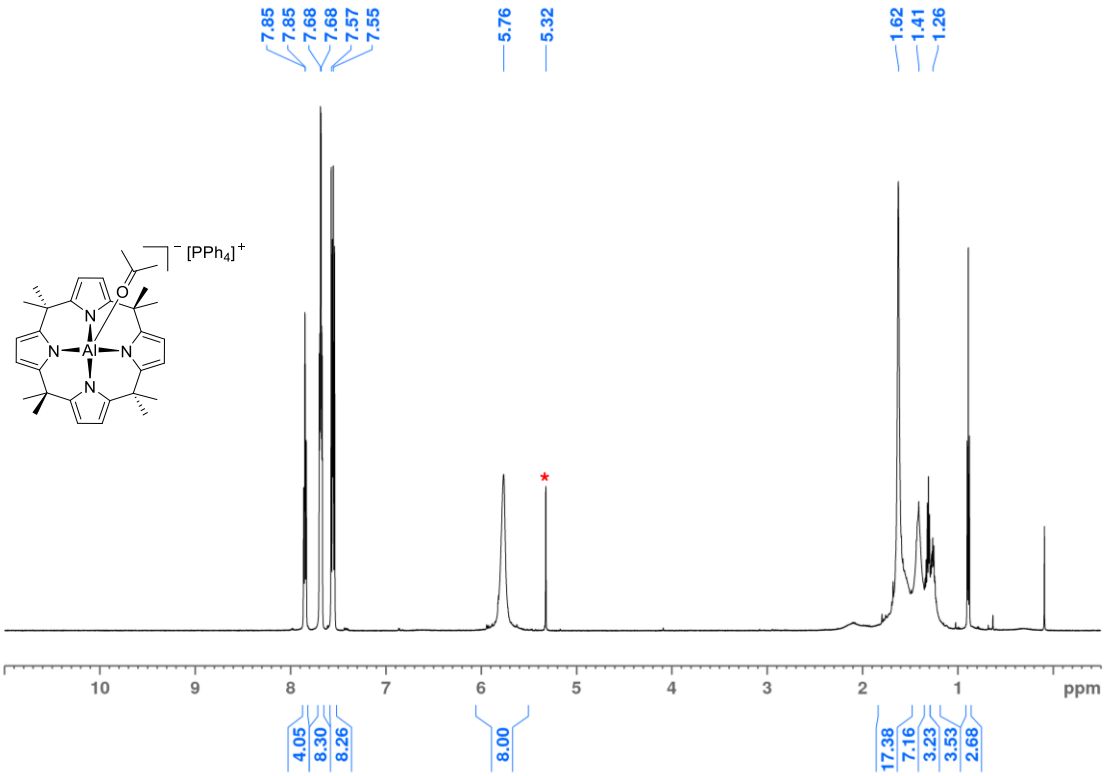


Figure S 87: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectrum of [PPh$_4$][**1**-acetone].

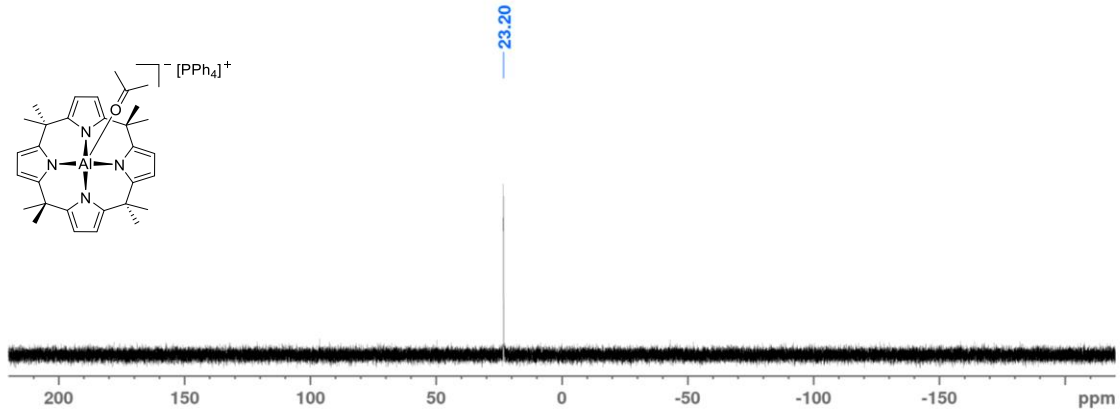


Figure S 88: ^{31}P NMR (243 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1**-acetone].

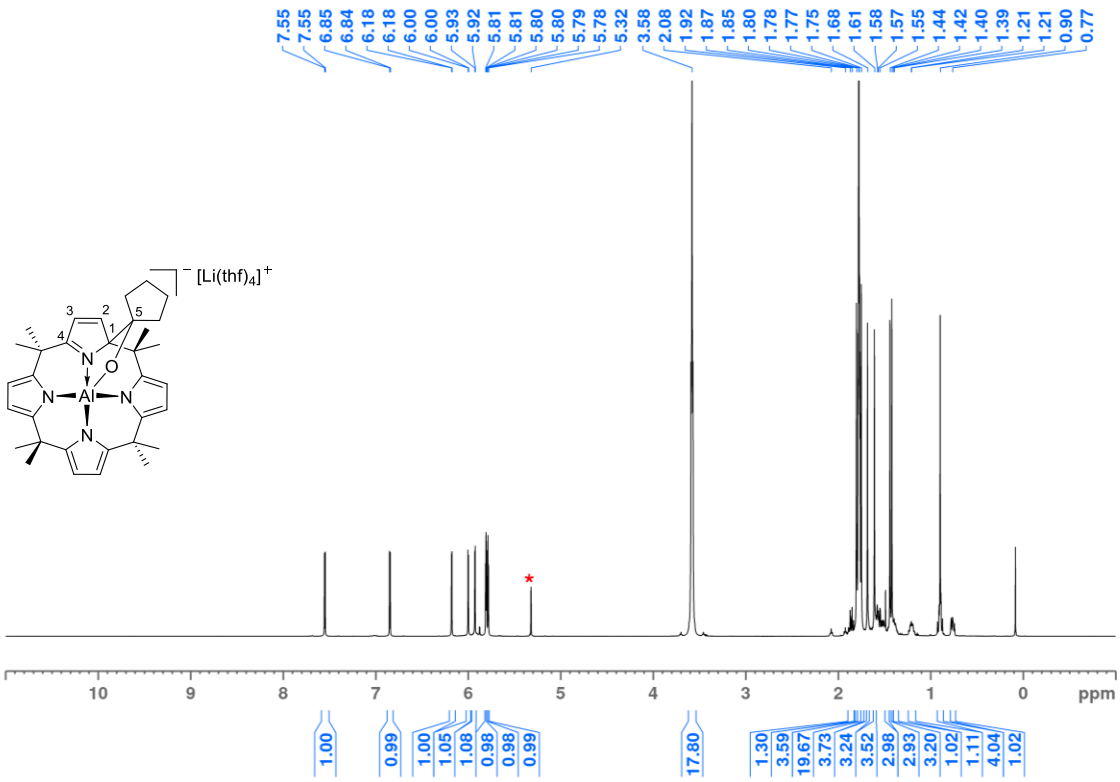


Figure S 89: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectrum of [$Li(thf)_4$][**1***-cyclopentanone].

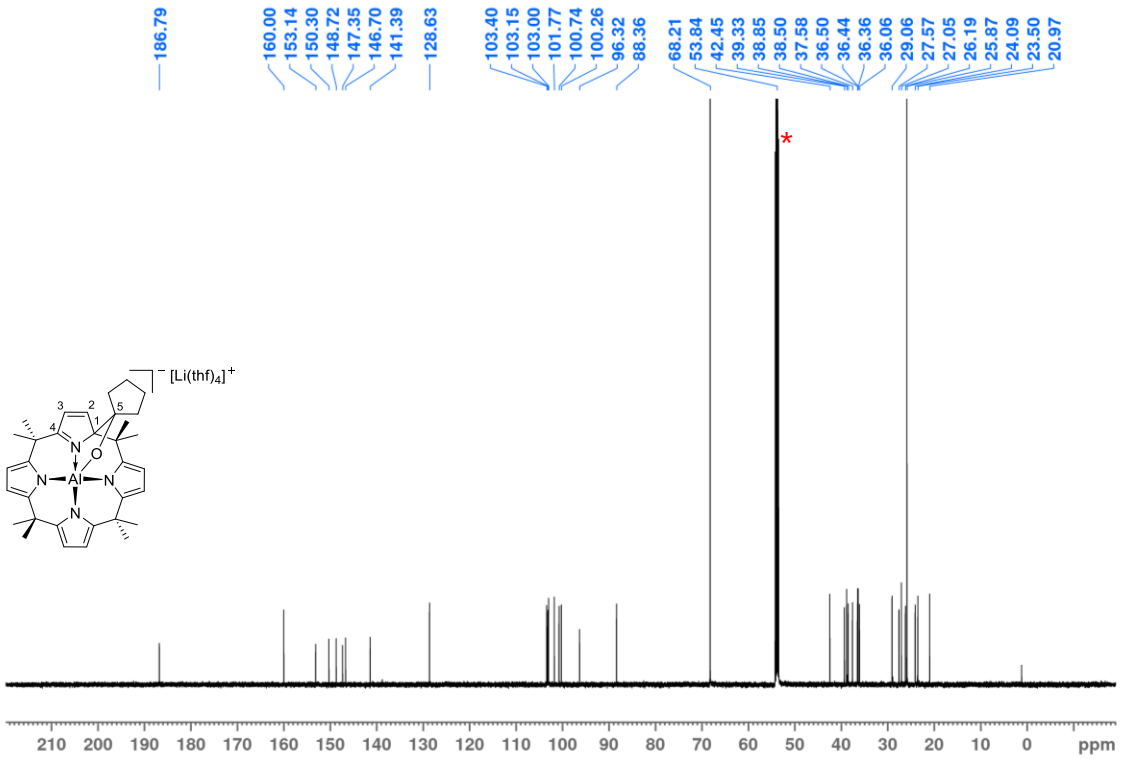


Figure S 90: $^{13}C\{^{1}H\}$ NMR (150 MHz, DCM-d_2, 295 K) spectrum of $[Li(thf)_4]$[**1***-cyclopenatanone].

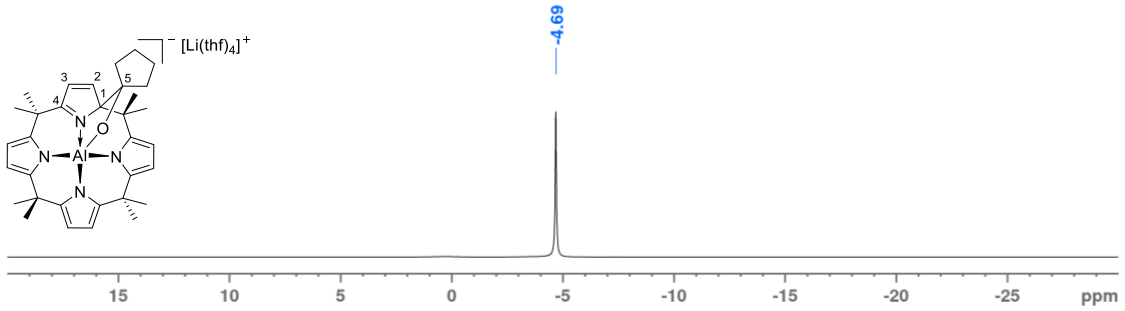


Figure S 91: ^{7}Li NMR (233 MHz, DCM-d_2, 295 K) spectrum of $[Li(thf)_4]$[**1***-cyclopentanone].

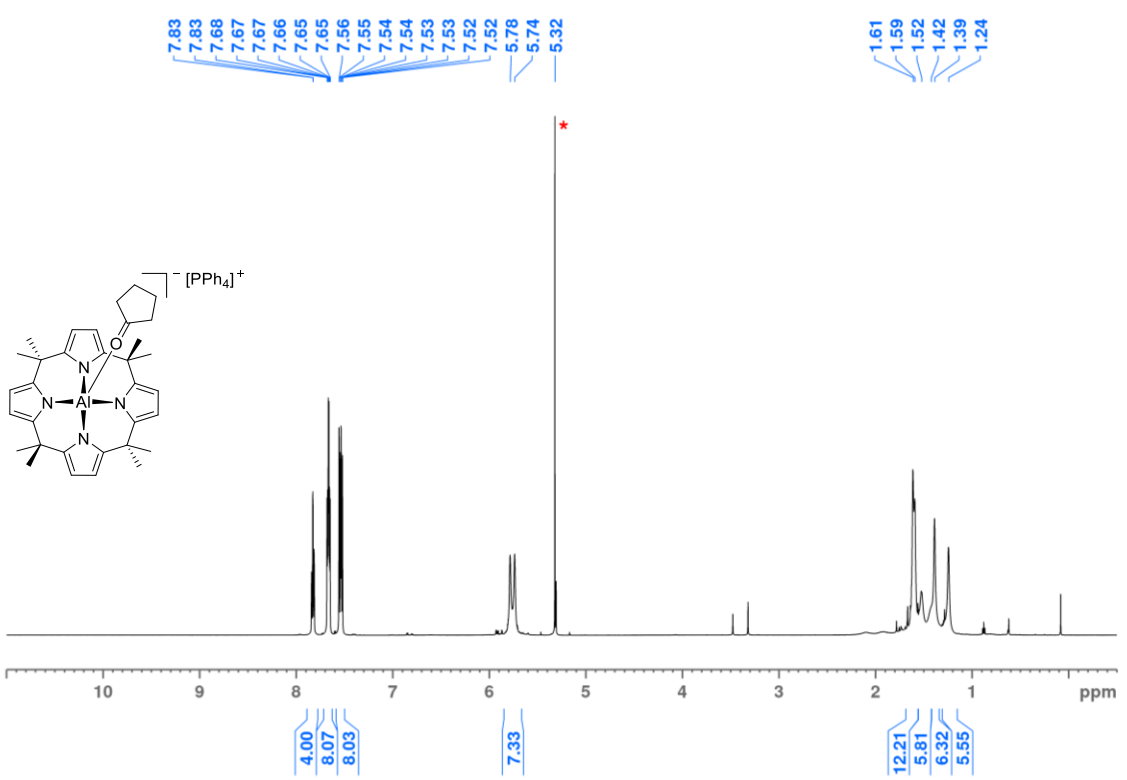


Figure S 92: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1**-cyclopentanone].

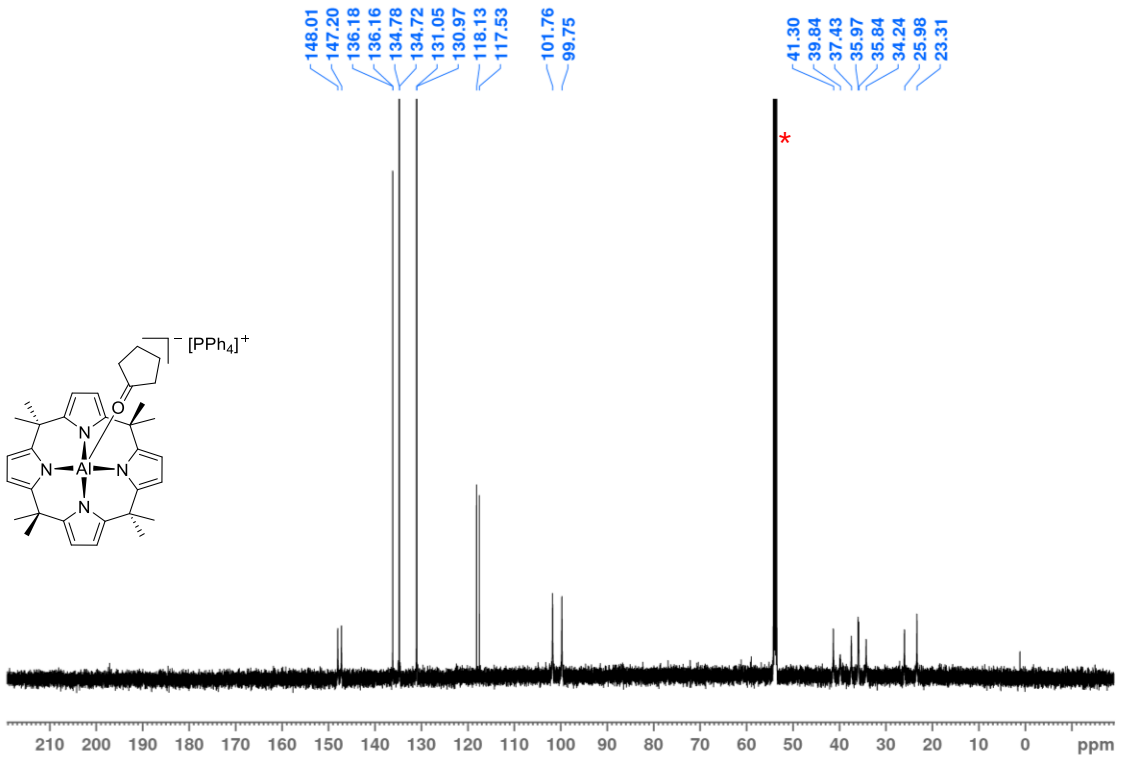


Figure S 93: $^{13}C\{^{1}H\}$ NMR (150 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1**-cyclopentanone].

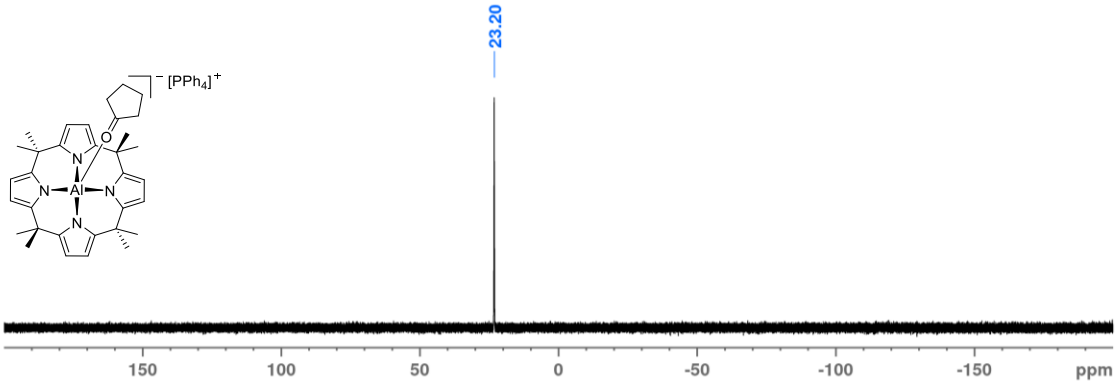


Figure S 94: ^{31}P NMR (243 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1**-cyclopentanone].

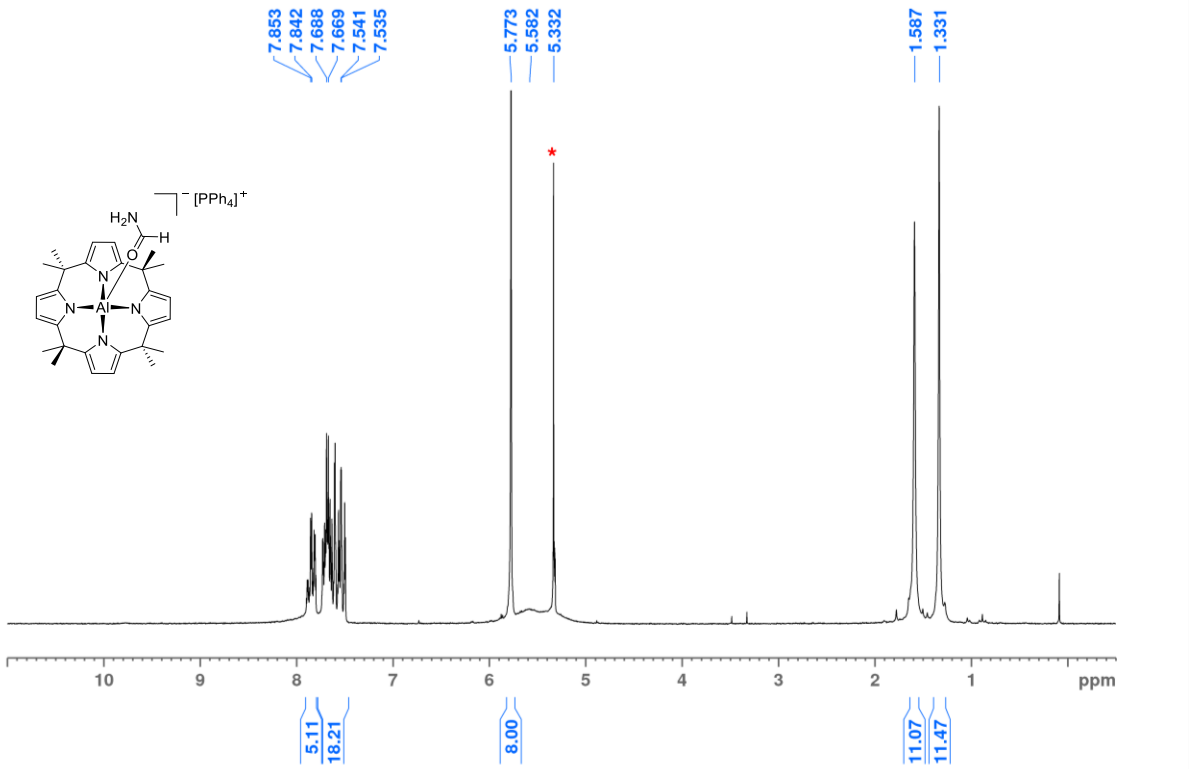


Figure S 95: ^{1}H NMR (200 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1**-formamide].

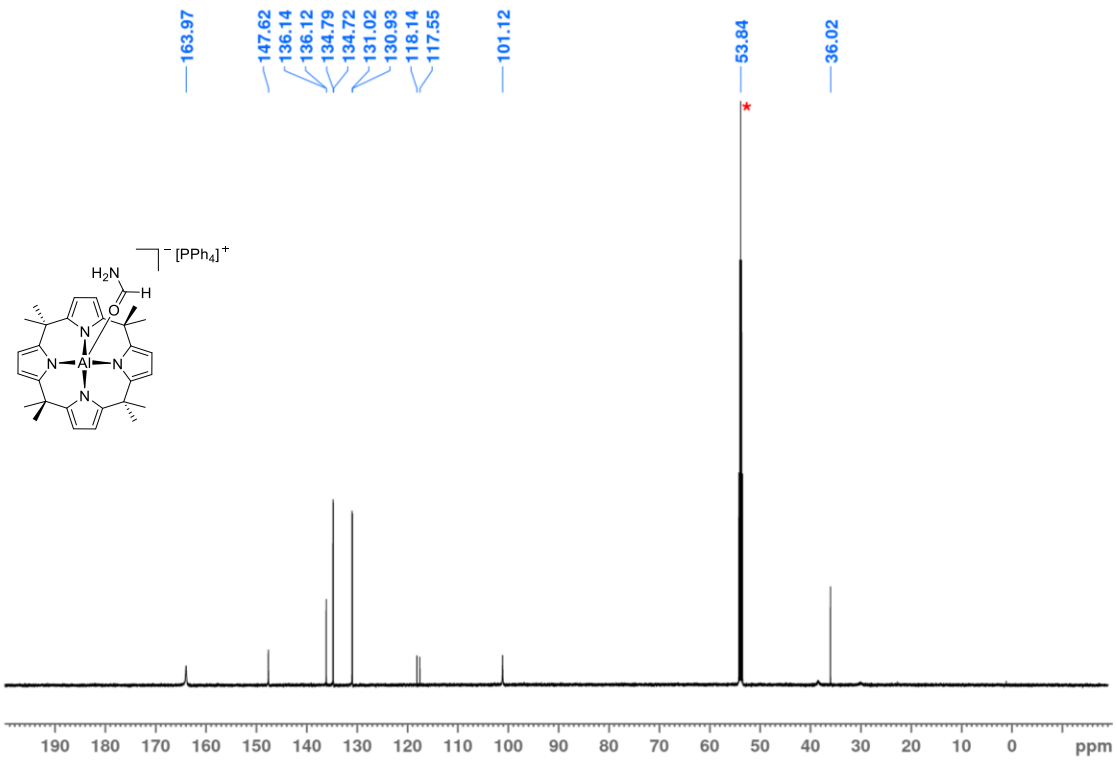


Figure S 96: $^{13}C\{^{1}H\}$ NMR (150 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1**-formamide].

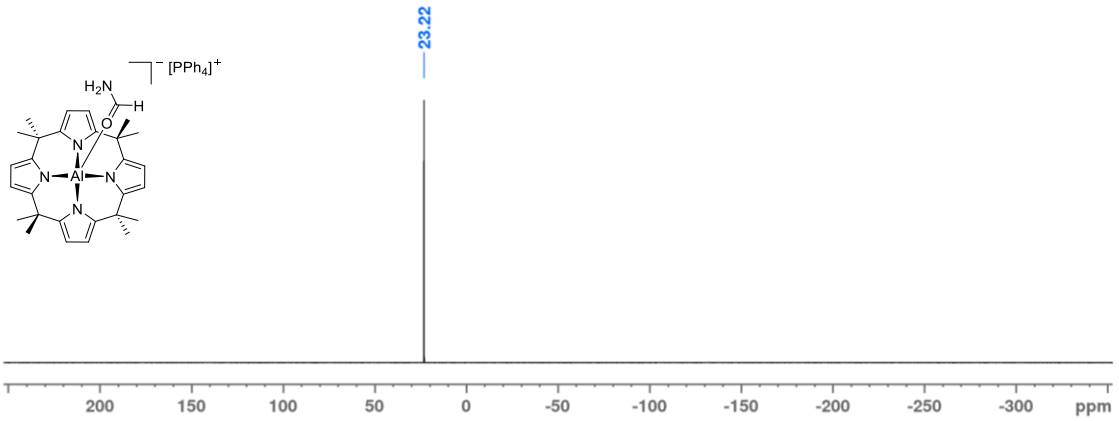


Figure S 97: ^{31}P NMR (243 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1**-formamide].

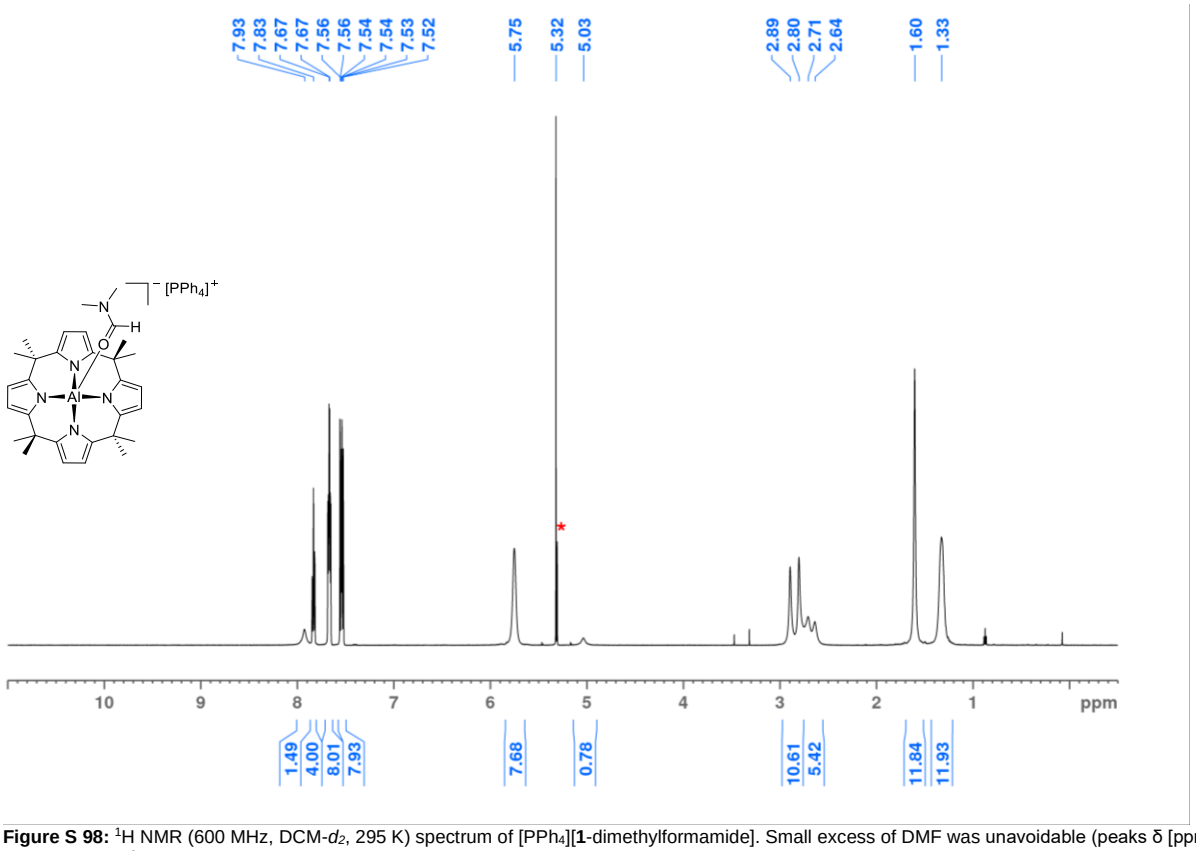


Figure S 98: ^{1}H NMR (600 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1**-dimethylformamide]. Small excess of DMF was unavoidable (peaks δ [ppm] = 2.80, 2.89, 7.93).

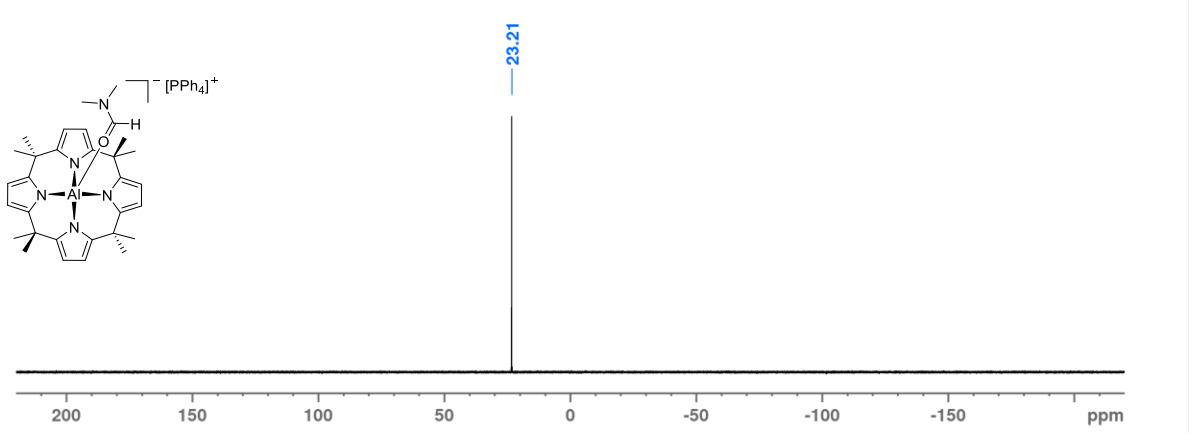


Figure S 99: ^{31}P NMR (243 MHz, DCM-d_2, 295 K) spectrum of [PPh_4][**1**-dimethylformamide].

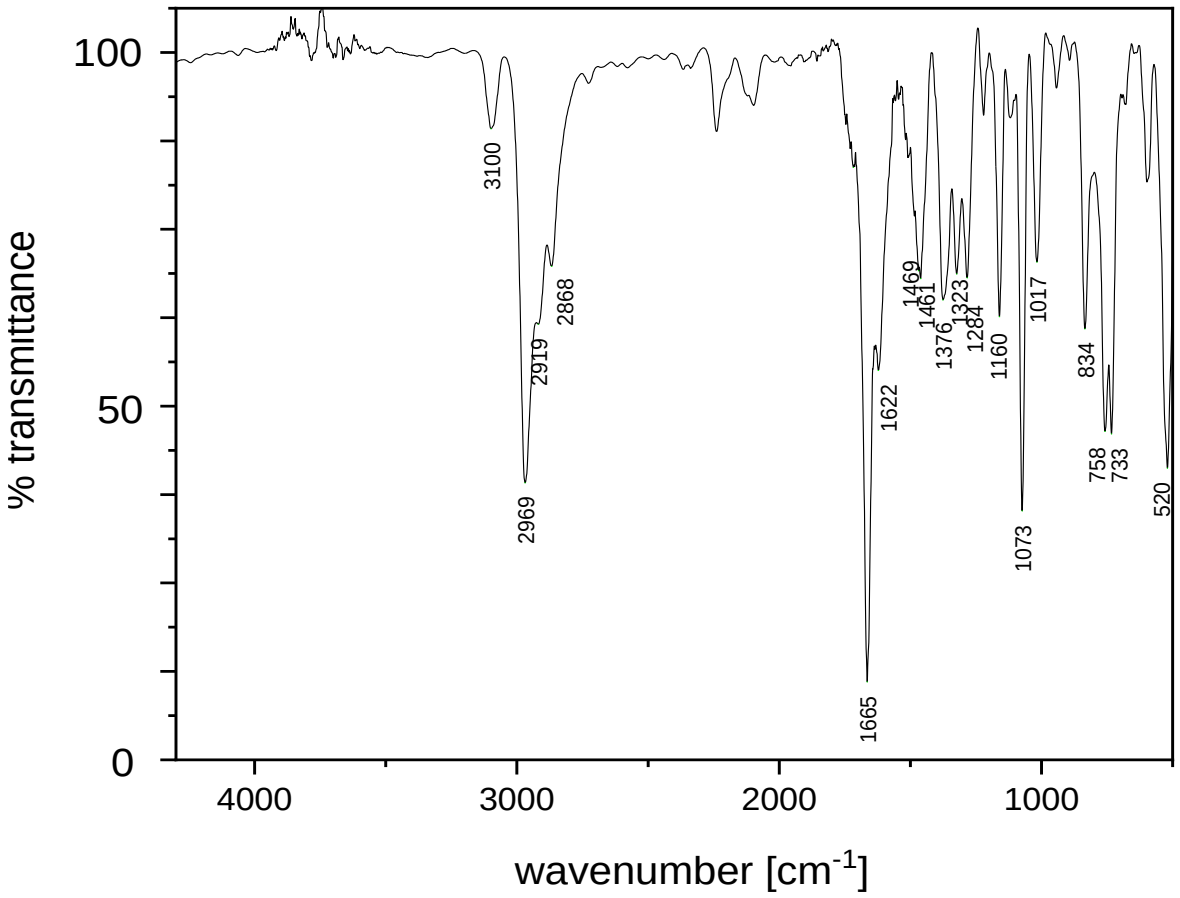


Figure S100. IR spectrum in KBr of $[Li(thf)_4][\mathbf{1}\text{-}CO_2]$. C=O band at $\tilde{\nu}$ = 1665 cm^{-1}.

12. Computational details

12.1. Geometry optimization and single point calculations

Geometry optimizations and single point energy calculations have been performed with ORCA 4.1.2.[2] The RI approximation[3] for the Coulomb integrals was used in all cases (RIJCOSX), with application of corresponding auxiliary basis sets. [4] The single point energies were obtained in two steps. The first geometry optimization was performed on Grimme's PBEh-3c composite method.[5] The obtained geometry was taken and single point energies were obtained on PW6B95-D3(BJ)/def2-QZVPP[6], including Grimme's semi-empirical dispersion correction[7] with Becke-Johnson damping function[8-10] (D3(BJ) def2-QZVPP[11] basis set).

All calculated geometries have been confirmed as energetic minima on the potential energy surface by analytical calculation of harmonic frequencies at the PBEh-3c level, revealing only positive Hessian eigenvalues. Enthalpies at 298.15 K have been calculated at the same level of theory by using the rigid-rotor harmonic oscillator (RRHO) approximation,[12] as implemented in ORCA. IRC calculations were performed on PBEh-3c level, confirming the transition states, as implemented in ORCA. Solvation free energies were obtained by COSMO-RS in dichloromethane as implemented in ADF[13].

12.2. Overview of different coordination modes and isomers: computation and spectroscopy

Different isomers of the adducts were found and taken into account during the calculations of the thermodynamics of the reactions and the transition states. These were also proofed by several analytical measurements. A rough overview and the connection between calculation and experiments are given now, followed by all computational details. The definition was done as followed and exemplarily shown for *p*DMA-BA (see figure S101): the σ-adduct-A is the one, in which the aldehyde proton points in the direction of the ligand and the opposite arrangement is called σ-adduct-B. The σ-adducts-A are generally computed more stable by roughly 20-30 kJ mol^{-1} in comparison to the σ-adducts-B (see figure S105), supporting the SCXRD result of σ-adduct-A for *p*DMA-BA (see figure 5B). However, the σ-adducts-A lead to the roughly 20 kJ mol^{-1} more unfavorable 1,2-adducts-A, due to the collision of the aldehyde residues with the methyl groups in the calix[4]pyrrolato backbone (see figure S101). In turn, the σ-adducts-B lead to more favorable 1,2-adducts-B, as has been observed in all cases by SCXRD (see figure. 3B). Nevertheless, the formation of all four isomers was detected for *p*DMA-BA by ^{1}H NMR spectroscopy (see section 5). Interestingly, in this case, the difference in computed free energies for the 1,2-adducts-A and B are closest in comparison with the other aldehydes (see figure S105).

For the calculation of the $[Li]^{+}$ salts, a single dimethoxyethane molecule was added to the structure for saturation of the Li cation. This motif was also found in various SCXDR structures. For obtaining correct solvent correction values $[Li]^{+}$ was calculated as $[Li(dme)_3]^{+}$. Furthermore, it was found by IRC that the σ-adduct A leads to the 1,2-adduct A and *vice versa*.

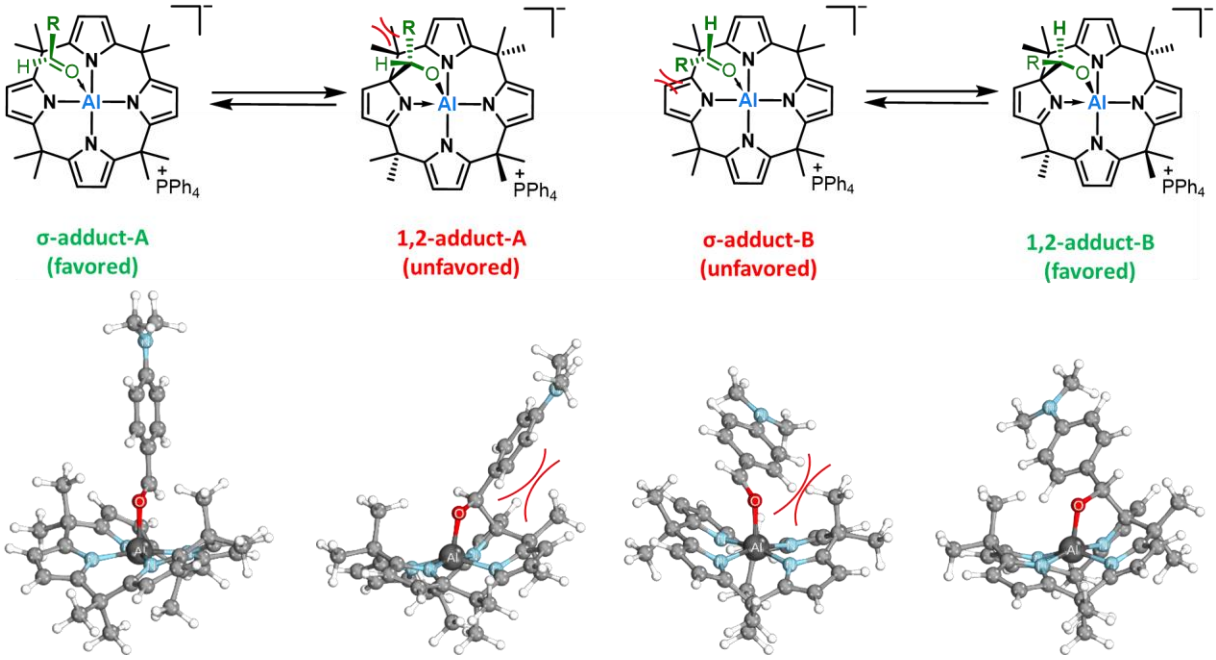


Figure S 101: Overview of the different possible adducts of $[PPh_4]$[**1**] and *p*-dimethylaminobenzaldehyde and nomenclature of the isomers.

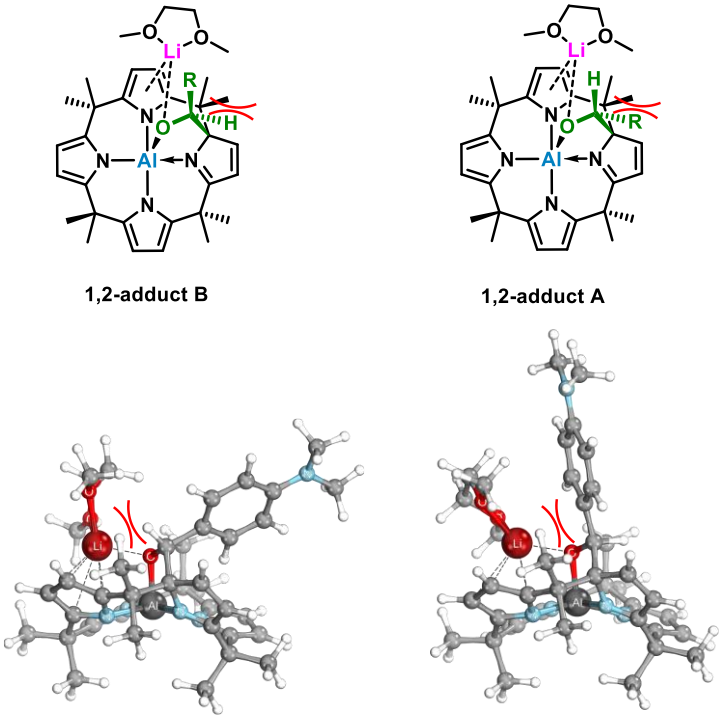


Figure S 102: Overview of the different adducts formed between [Li(dme)][**1**] and *p*-dimethylaminobenzaldehyde.

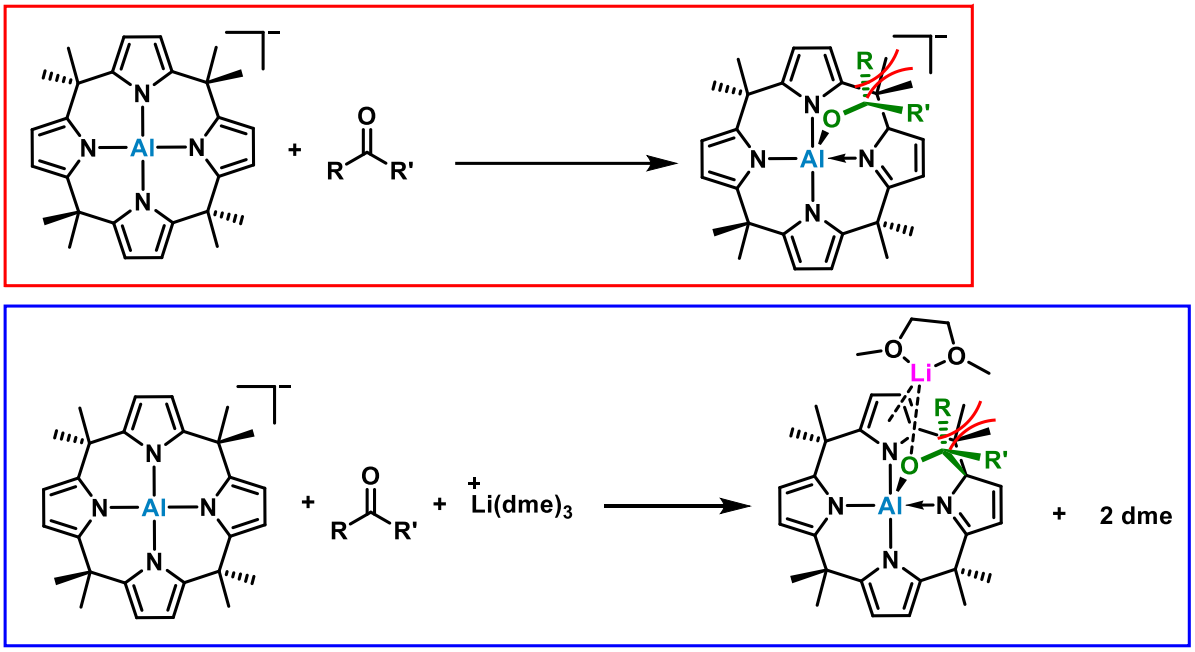


Figure S 103: Reactions, that led to $\Delta_r G$ in Figure S 104. All calculations are minimum structures on PBEh-3c and SP energies are calculated on PW6B95/QZVPP level of theory. Solvent correction was performed with COSMO-RS for dichloromethane in ADF. Colors merge with those in figure S 104.

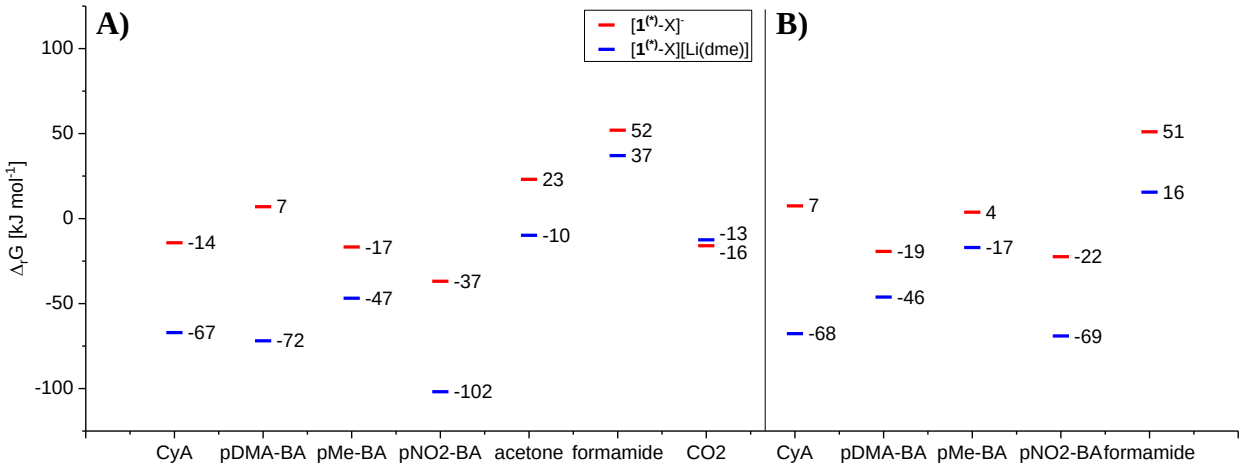


Figure S 104: Overview of the free reaction enthalpies for the reactions shown in figure S 103. Red lines: σ-adducts / Blue lines 1,2-adducts + $Li(dme)^+$ **A**) shows isomer B, **B**) isomer A.

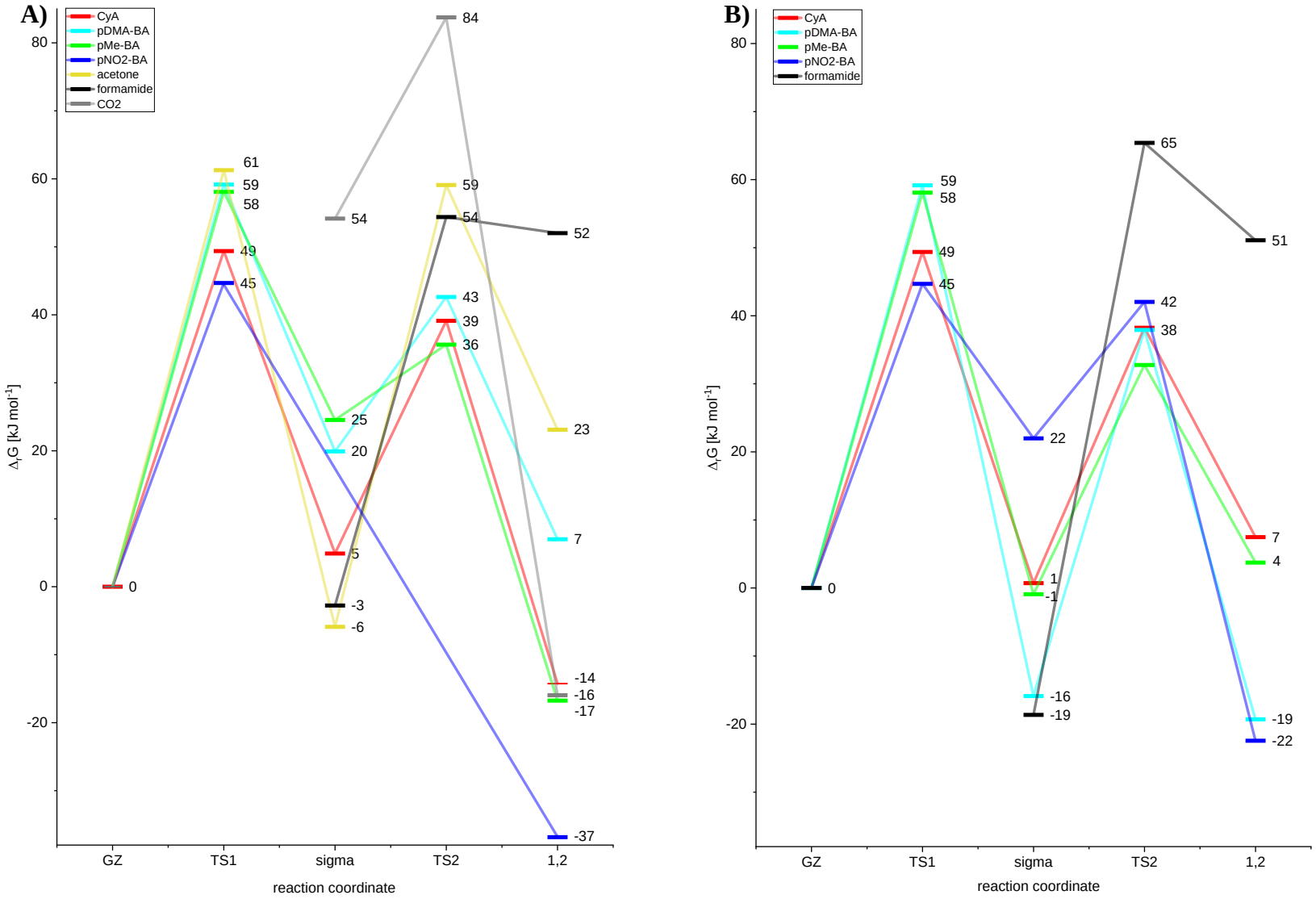


Figure S 105: Reaction coordinate for the formation of the □-adduct and the subsequent 1,2-addition product generation calculated on the PW6B95-D3(BJ), COSMO-RS(CH_2Cl_2)/def2-QZVPP//PBEh-3c level of theory. Energies were calculated for both isomers **A**) isomer B and **B**) isomer A.

13. X-ray Crystal Structure Determinations

Crystal data and details of the structure determinations are compiled in the following tables. Intensity data were collected at low temperature with an Enraf Nonius Kappa CCD diffractometer (Mo-K_α radiation, sealed X-ray tube, graphite monochromator), or a Bruker AXS D8 Venture diffractometer (Mo-K_α radiation, microfocus X-ray tube, multilayer mirror optics). Data were processed with the standard Nonius and Bruker (SAINT, APEX3) software package.[14] Multiscan absorption correction was applied using the SADABS program.[15] The structures were solved by intrinsic phasing[16] and refined using the SHELXTL software package (Version 2018/3).[17] Graphical handling of the structural data during solution and refinement were performed with OLEX2.[18] All non-hydrogen atoms were given anisotropic displacement parameters. Hydrogen atoms were generally input at calculated positions and refined with a riding model. When justified by the quality of the data the positions (and sometimes isotropic temperature factors) of some hydrogen atoms were refined. Split atom models were used to refine disordered groups and/or solvent molecules. The dataset collected for [$Li(thf)_2$][**1***-acetone] was not of sufficient quality to warrant detailed publication. However, these structures could be solved and the molecular connectivity unambiguously established. Due to severe disorder and fractional occupancy, electron density attributed to solvent of crystallization was removed from the structures of [**1***-CO_2][PPh_4] (dichloromethane), [**1***-dimethylformamide][PPh_4] (dichloromethane and pentane), [**1***-formamide][PPh_4] (dichloromethane) and [**1***-*p*-Dimethylaminobenzaldehyde][$Li(thf)_2$] (dichloromethane) with the BYPASS procedure,[19] as implemented in PLATON (squeeze/hybrid).[20] Partial structure factors from the solvent masks were included in the refinement as separate contributions to F_{calc}. CCDC 1989029-1989036 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre's and FIZ Karlsruhe's joint Access Service via https://www.ccdc.cam.ac.uk/structures/?.

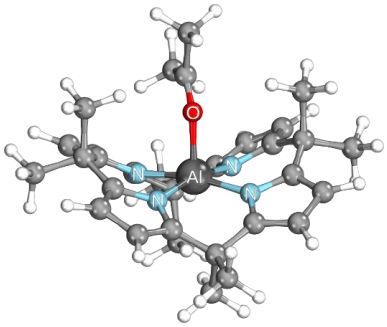
Identification code	[**1***-Cyclohexanecarboxaldehyde][PPh_4]	[**1**-*p*-Dimethylaminobenzaldehyde][PPh_4]	[**1***-*p*-Nitrobenzaldehyde][PPh_4]
Empirical formula	$C_{66}H_{72}AlN_4OP$	$C_{63}H_{67}AlCl_4N_5OP$	$C_{60}H_{59}AlCl_2N_5O_3P$
Formula weight	995.22	1109.96	1026.97
Temperature/K	121.0	100.0	100.0
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1$	$P2_1/n$	$P2_1/c$
a/Å	11.5021(5)	20.180(6)	15.1362(10)
b/Å	17.7007(7)	13.614(3)	16.5731(10)
c/Å	14.3727(7)	22.998(8)	21.0581(13)
α/°	90	90	90
β/°	113.240(2)	113.063(14)	104.851(3)
γ/°	90	90	90
Volume/$Å^3$	2688.8(2)	5813(3)	5106.0(6)
Z	2	4	4
$\rho_{calc}g/cm^3$	1.229	1.268	1.336
μ/mm^{-1}	0.116	0.292	0.229
F(000)	1064.0	2336.0	2160.0
Crystal size/mm^3	0.35 × 0.2 × 0.2	0.145 × 0.105 × 0.069	0.26 × 0.13 × 0.1
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.848 to 60.156	4.388 to 58	3.714 to 58.284
Index ranges	-16 ≤ h ≤ 16, -24 ≤ k ≤ 24, -20 ≤ l ≤ 20	-27 ≤ h ≤ 27, -18 ≤ k ≤ 18, -31 ≤ l ≤ 31	-20 ≤ h ≤ 20, -22 ≤ k ≤ 22, -28 ≤ l ≤ 28
Reflections collected	122966	164437	227435
Independent reflections	15758 [R_{int} = 0.0702, R_{sigma} = 0.0523]	15455 [R_{int} = 0.1530, R_{sigma} = 0.0708]	13720 [R_{int} = 0.0933, R_{sigma} = 0.0319]
Data/restraints/parameters	15758/1/667	15455/3/699	13720/0/657
Goodness-of-fit on F^2	1.059	1.022	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0408, wR_2 = 0.1001	R_1 = 0.0607, wR_2 = 0.1254	R_1 = 0.0398, wR_2 = 0.0874
Final R indexes [all data]	R_1 = 0.0607, wR_2 = 0.1058	R_1 = 0.1134, wR_2 = 0.1591	R_1 = 0.0604, wR_2 = 0.0990
Largest diff. peak/hole / e $Å^{-3}$	0.43/-0.34	0.95/-1.07	0.56/-0.65
Flack parameter	0.01(3)		
CCDC deposition number	1989032	1989036	1989033

Identification code	[**1***-*p*-Dimethylaminobenzaldehyde][Li(thf)$_2$]	[**1***-dimethylformamide][PPh$_4$]	[**1**-formanide][PPh$_4$]	[**1***-CO$_2$][PPh$_4$]
Empirical formula	$C_{45}H_{59}AlLiN_5O_3$	$C_{55}H_{59}AlN_5OP$	$C_{54}H_{57}AlCl_2N_5OP$	$C_{57}H_{60}N_4O_3AlP$
Formula weight	751.89	864.02	920.89	907.04
Temperature/K	100.0	100.0	293.15	120
Crystal system	orthorhombic	triclinic	triclinic	triclinic
Space group	$P2_12_12_1$	P-1	P-1	P-1
a/Å	8.6388(3)	12.1492(6)	11.527(16)	10.923(2)
b/Å	20.8824(7)	14.4072(7)	12.360(17)	14.476(3)
c/Å	24.1541(8)	16.3459(9)	19.11(3)	18.472(4)
α/°	90	80.033(2)	90.58(6)	87.06(3)
β/°	90	88.754(2)	92.72(6)	80.80(3)
γ/°	90	65.193(2)	106.31(4)	68.01(3)
Volume/Å^3	4357.4(3)	2553.8(2)	2609(7)	2673.5(11)
Z	4	2	2	2
ρ_{calc}g/cm^3	1.146	1.124	1.172	1.127
μ/mm^{-1}	0.090	0.113	0.213	0.113
F(000)	1616.0	920.0	972.0	964.0
Crystal size/mm^3	0.199 × 0.192 × 0.148	0.23 × 0.13 × 0.12	0.212 × 0.2 × 0.135	0.35 × 0.2 × 0.15
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.896 to 61.094	3.7 to 55.098	4.088 to 55.038	4.068 to 49.998
Index ranges	-12 ≤ h ≤ 12, -28 ≤ k ≤ 29, -34 ≤ l ≤ 34	-15 ≤ h ≤ 15, -18 ≤ k ≤ 18, -21 ≤ l ≤ 21	-14 ≤ h ≤ 14, -16 ≤ k ≤ 16, -24 ≤ l ≤ 24	-12 ≤ h ≤ 12, -17 ≤ k ≤ 17, -21 ≤ l ≤ 21
Reflections collected	185155	90418	117792	16040
Independent reflections	13335 [R_{int} = 0.0572, R_{sigma} = 0.0244]	11733 [R_{int} = 0.0844, R_{sigma} = 0.0441]	11945 [R_{int} = 0.0598, R_{sigma} = 0.0271]	9230 [R_{int} = 0.0934, R_{sigma} = 0.1816]
Data/restraints/parameters	13335/5/529	11733/0/578	11945/0/593	9230/0/603
Goodness-of-fit on F^2	1.034	1.029	1.069	0.953
Final R indexes [I>=2σ (I)]	R_1 = 0.0335, wR_2 = 0.0842	R_1 = 0.0487, wR_2 = 0.1223	R_1 = 0.0431, wR_2 = 0.1011	R_1 = 0.0689, wR_2 = 0.1499
Final R indexes [all data]	R_1 = 0.0386, wR_2 = 0.0875	R_1 = 0.0665, wR_2 = 0.1353	R_1 = 0.0537, wR_2 = 0.1069	R_1 = 0.1859, wR_2 = 0.1926
Largest diff. peak/hole / e Å^{-3}	0.23/-0.18	0.51/-0.46	0.62/-0.99	0.24/-0.25
Flack parameter	0.13(3)			
CCDC deposition number	1989030	1989031	1989034	1989029

Identification code	[**1***-*p*-Methylbenzaldehyde][PPh_4]
Empirical formula	$C_{60}H_{60}AlN_4OP$
Formula weight	911.07
Temperature/K	120
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.516(2)
b/Å	26.230(5)
c/Å	18.872(4)
α/°	90
β/°	97.34(3)
γ/°	90
Volume/$Å^3$	5654(2)
Z	4
$\rho_{calc}g/cm^3$	1.070
μ/mm^{-1}	0.105
F(000)	1936.0
Crystal size/mm^3	0.2 × 0.18 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.408 to 55
Index ranges	-14 ≤ h ≤ 14, -32 ≤ k ≤ 34, -24 ≤ l ≤ 24
Reflections collected	25253
Independent reflections	12950 [R_{int} = 0.1301, R_{sigma} = 0.1850]
Data/restraints/parameters	12950/0/613
Goodness-of-fit on F^2	0.919
Final R indexes [I>=2σ (I)]	R_1 = 0.0652, wR_2 = 0.1316
Final R indexes [all data]	R_1 = 0.1747, wR_2 = 0.1650
Largest diff. peak/hole / e $Å^{-3}$	0.26/-0.32
CCDC deposition number	1989035

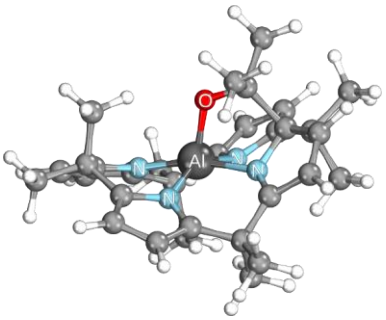
14. **Appendix**

Calculated molecular structures (PBEh-3c)



[**1**$^-$]-acetone sigma adduct

N	-0.18339812152414	-2.18398769078147	0.35021274112398
C	-0.85769550386692	-3.20968480862822	0.96867825107548
C	0.19304186043066	-2.63274775512337	-0.88471627609443
C	-0.94645804538349	-4.27899722279143	0.10141736330744
H	-1.40134784653133	-5.23655912948497	0.30528063270965
C	-0.26700556996119	-3.91299729536645	-1.08172816470665
H	-0.11567150405548	-4.52751466952192	-1.95569785890834
N	-0.12923256693252	-0.97098785913065	2.74680536887963
C	0.41620687581706	-0.29904790110117	3.80826616580689
C	-0.64440744256709	-2.14717935651228	3.23759595466179
C	0.22713135415756	-1.01604942500312	4.96395203696507
C	-0.45503888754747	-2.19548213036022	4.59941283864308
H	-0.75724355072084	-2.98880712282420	5.26563393911938
N	0.02513427798074	1.50901835494243	1.49700775705913
C	-0.34007070281553	2.64753984118995	0.81862601679828
C	0.56049576614872	1.90971266073609	2.69230850674634
C	-0.06749080780506	3.74949396205570	1.59578807142400
H	-0.25052349606728	4.78157563442733	1.33935730950275
C	0.51245764043831	3.27835328760030	2.79202860571452
H	0.87159981083114	3.87910886688103	3.61293662532356
N	-0.03349741314089	0.30991879354561	-0.90596407059216
C	0.31817894008490	-0.45402193678509	-1.98396618502259
C	-0.57701523261061	1.47497282630536	-1.39205144719631
C	-0.03294763454782	0.18600220281376	-3.14930369073520
H	0.12931868424805	-0.16826725200894	-4.15558367256870
C	-0.61222397755321	1.41674669886370	-2.76948432011146
H	-0.96769067629653	2.18690648675164	-3.43710493965107
H	0.25015827627525	-2.65254567393069	-3.63306859260886
C	1.20543720037912	-2.46007622909870	-3.14352661708493
C	2.41081948203209	-1.54031047335983	-1.18392113825583
C	1.01542518131935	-1.76942461872805	-1.79590501392384
H	2.92574165408716	-2.49231467651135	-1.03937479861779
H	1.72028359849363	-3.41334561854001	-3.01578665023998
H	2.35910770477631	-1.04839596479638	-0.21234120288760
H	-3.18589569139647	-2.00978414099009	2.29380517380403
C	-2.86967700403463	-3.02735231286688	2.50584976711206
C	-1.01659757845628	-4.57751925911500	3.00454550621273
C	-1.33687419094278	-3.19547076727712	2.40429658274306
H	0.05183128094667	-4.78137966724798	2.95978538279895
H	-3.38510367049425	-3.70796626117960	1.82327827413946
H	-1.53945790942541	-5.36852687659405	2.46537086650138
H	3.23012361226457	1.42249186270032	2.85261470929073
C	2.60348107758127	0.54041529374554	3.00080083703130
C	1.51604432631271	1.60159111588659	4.95925234544583
C	1.24128729045179	0.93833276923580	3.61083628845610
H	2.04370505548981	0.91723804083485	5.62473726749396
H	2.48792748930183	0.05666044517651	2.02961315908514
H	0.58993894674905	1.90799371471184	5.44568141669098
C	-0.97768603624622	2.66490594067398	-0.54720649388891
C	-2.51160840745938	2.79599661877169	-0.41437805717476
C	-0.50163507798511	3.92948641612084	-1.28671849248017
H	-2.99880659258099	2.69904543255347	-1.38799303699327
H	-0.98005475373821	4.01407646273162	-2.26330272113358
H	-2.92811844612822	2.05639638028130	0.26347401319196
H	0.57672771560306	3.90972710403578	-1.43446394223332
H	-2.76574142417614	3.77315501929571	0.00146575306841
H	-0.75685793526939	4.83021042364568	-0.72774707515797
H	3.01566806759939	-0.90757433756851	-1.83672466108571
H	1.80997018425280	-1.84169646399021	-3.80856658065943
H	-1.33555353600478	-4.63654809646048	4.04551704789932
H	-3.20033022976925	-3.24610393584157	3.52324513146440
H	2.14623073218300	2.48297986994449	4.83400506790824
H	3.12603072107870	-0.16172444891652	3.65398076509626
H	0.55879199906081	-0.74479917108330	5.95400414014981
Al	-0.29630391888248	-0.31630557193331	0.93029598468056
O	-2.24747616960241	-0.23902838493298	0.84470570194310
C	-3.12474479608025	-0.59196447176790	0.06547955251609
C	-2.87300970385342	-1.30839317284306	-1.21082113046896
H	-2.16206733461097	-0.76161718798195	-1.83457300565627
H	-3.79856057110134	-1.45947580399365	-1.76324601860975
H	-2.41785101270321	-2.28254357030262	-1.00505948909315
C	-4.54676984167800	-0.29606693877109	0.41956018749832
H	-4.62904124992310	0.19665766021156	1.38461912736276
H	-5.11909558308785	-1.22591821613296	0.42748923982866
H	-4.98264121081756	0.33828869150890	-0.35543612243355



[**1**$^-$]-acetone 1,2 adduct

N	-0.16832396684232	-2.21960194672633	0.30660277283891
C	0.26337131201928	-3.17746872437028	1.18730727324562
C	-0.44256960273859	-2.85448114463988	-0.87347839523542
C	0.26824108961520	-4.40960168104196	0.57448171494810
H	0.56680469260707	-5.35083437308623	1.01087735618025
C	-0.18359699351348	-4.20249225453221	-0.74594028682017
H	-0.30757719102218	-4.95920031711576	-1.50457311684282
N	-0.58994990461377	-0.84622921673499	2.53239253980423
C	-1.61136836597666	-0.09554527059209	3.20839848527030
C	-0.27966741200311	-1.90146216498892	3.18159692585941
C	-1.85784643126926	-0.90774223767712	4.43445384223405
C	-1.05113807059456	-1.97976517777730	4.41952515977326
H	-0.99337349928607	-2.77123266016918	5.15128429198401
N	0.07564470171648	1.44743147566800	1.23558374647937
C	0.43752292254319	2.44985499395216	0.37928724954804
C	-0.57365059458595	2.04320002949520	2.29382076014179
C	0.03297292586886	3.66626678209614	0.87699755877843
H	0.18130480302831	4.63344907056335	0.42277664571509
C	-0.62012582814012	3.40405786317495	2.10268746469465
H	-1.04765809256396	4.13764023428411	2.76977182109498
N	-0.06993906073324	0.04076496717050	-1.22634652851849
C	-0.35718270825898	-0.80042294114182	-2.26977350066233
C	0.56583244867605	1.13666568264753	-1.74270581023211
C	0.06510991913280	-0.22728940389030	-3.44607119821063
H	-0.02385673644199	-0.64525516175641	-4.43689298028244
C	0.65736954888232	1.01133670250218	-3.10882415557941
H	1.11840179410981	1.70845195893206	-3.79174499918615
H	-2.79604894494279	-1.33895435897271	-1.01921219866577
C	-2.55237888175039	-1.95641695337317	-1.88057092138641
C	-0.82840315050595	-2.99264337823544	-3.31709543192736
C	-1.03035741279897	-2.13420134443453	-2.06599449906574
H	-1.33309117307721	-3.95399511395398	-3.21066484723249
H	-3.03190193879427	-2.92934561214149	-1.74565683500884
H	0.22837312612879	-3.17628670514472	-3.51015921517572
H	-0.13479089261338	-4.65218830397396	3.48183978880739
C	0.81711543844836	-4.12203083188005	3.43839690457023
C	2.09619648668223	-2.16470205507624	2.57510859378153
C	0.71876907238174	-2.85511379860075	2.59272364623358
H	2.08236075682195	-1.25665460553320	1.97319716234358
H	1.55680455155119	-4.80162153222333	3.01658403697556
H	2.83235629893806	-2.84054620550289	2.13914325421023
H	1.09206399587160	0.52813117114900	3.78601645383548
C	0.34374172072097	1.07696035173380	4.35321769513166
C	-1.85271621610671	2.15679714242067	4.44973386911981
C	-0.95727927714034	1.30040584312809	3.54771826373700
H	-2.12904798071628	1.61695061832555	5.35739680252177
H	0.17143219953421	0.55958008681922	5.30018133758537
H	-2.76170570459354	2.49905699374987	3.96707095249298
C	1.23484610950022	2.15958487146183	-0.86090882833498
C	1.45973291948239	3.45145784514264	-1.64499589399876
C	2.61601023926401	1.61237186622663	-0.43993669867833
H	2.08416081535227	3.26782087979846	-2.51985743157427
H	3.23284911011987	1.41805709925027	-1.31963744810222
H	0.51556209752392	3.87634903288067	-1.98567760989261
H	2.51825627622398	0.67469224785297	0.10749780372175
H	1.97092277281238	4.19295434288236	-1.02852965728248
H	3.13500264971184	2.32477776651642	0.20623814418327
H	-1.25751162727126	-2.50023094236254	-4.19056114394683
H	-2.98001452970452	-1.47757946098037	-2.76455635103675
H	2.42534271350102	-1.89552195260077	3.58263931033182
H	1.13377496581343	-3.88909808346292	4.45743081686690
H	-1.30153899126389	3.04240822959208	4.76717818035640
H	0.77334302848711	2.05341620516457	4.57766183164588
H	-2.57382407670481	-0.65818251136888	5.20419286175034
Al	-0.54538098159390	-0.30080307818829	0.59259597295139
O	-2.28887963943307	-0.02366026935219	0.86442322245572
C	-2.81764950310320	-0.14351616881016	2.12732612171287
C	-3.85221292087846	0.95873188929335	2.33862385587553
H	-3.42481598279092	1.93658829246935	2.12357811306899
H	-4.27751560897898	0.95669325170465	3.34494008560707
H	-4.66903328931205	0.79860333498254	1.63246062338371
C	-3.52728480616209	-1.50201776906272	2.24544128616744
H	-2.83742424740444	-2.33944074341773	2.13313033263248
H	-4.24820391831238	-1.57327062082559	1.42965851529403
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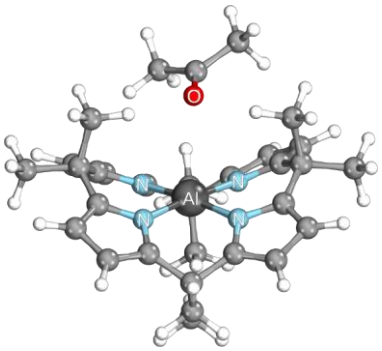

[**1**$^-$]-acetone TS 1

N	0.85649322594930	-0.73191915520189	1.80569927400644
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C	0.62642396887127	-1.13247502976856	3.09697886177701
C	2.77348426450377	-0.53208043056816	2.95194034719401
H	3.80425237726472	-0.33282044101080	3.19959603019045
C	1.78196245760496	-1.02813872367731	3.82937020050401
H	1.91100148455920	-1.27970996936653	4.87059590836277
N	0.99646105039064	-1.00508405297581	-0.86152845078705
C	0.89278491888673	-1.68037322656927	-2.05499202473475
C	2.31528028002147	-0.63558788235089	-0.72628621870179
C	2.11376692277442	-1.71575218233898	-2.67609279012120
C	3.02258808698888	-1.04213587760254	-1.82821536227185
H	4.07416255553920	-0.88638818156846	-2.01099631956151
N	-1.74080697273895	-0.86776992078116	-1.01845538478178
C	-3.02634792798331	-0.37440062149398	-1.02882656408177
C	-1.57654440945499	-1.57656731449245	-2.18534351708206
C	-3.65083225833294	-0.74785528806622	-2.19189777988534
H	-4.65627497475086	-0.49769890041335	-2.49176486793328
C	-2.72606211213623	-1.52025792095166	-2.92903192434235
H	-2.90023578281523	-1.99373095756209	-3.88244739076473
N	-1.88683506562983	-0.52397813987447	1.63369784260820
C	-1.81185812521470	-0.79812952049381	2.97402668427328
C	-3.08361097905827	0.11339560094278	1.40946220840837
C	-2.92934240953474	-0.31459245471569	3.60890784890107
H	-3.16741686338458	-0.40912718981891	4.65722658760458
C	-3.74143477848542	0.26974047991543	2.60836555707208
H	-4.71117955809135	0.71955778299068	2.75614461943156
H	-0.67621326555603	-0.72305682725269	5.48625079810483
C	-0.79539285904815	-1.71331268257679	5.04529019502383
C	-0.88952150229786	-3.10365561524839	2.99849552274931
C	-0.71205245785535	-1.66231946128440	3.52144134660296
H	-0.10364666702382	-3.75143208794638	3.39172531663016
H	-0.01805769379663	-2.36096085817456	5.45225159863057
H	-0.83734009206355	-3.15725739305915	1.90962939046918
H	1.50127412678398	1.85527164464032	0.07027404236013
C	2.55212945087562	1.64646470913045	0.24029647821484
C	4.33787057983543	-0.02799471926447	0.56459810619419
C	2.81967395156235	0.14195355864039	0.45571015841595
H	4.61314214231789	-1.07159838627389	0.71283350516273
H	2.87139190248748	2.22356138528210	1.11046672770451
H	4.73128146923667	0.55562351428157	1.39811806390598
H	-1.35888115363098	-4.26460214268472	-1.84724853585801
C	-0.45646783500750	-3.70648439556309	-1.58988773106736
C	-0.29851109213785	-2.82712143695483	-3.90230207338505
C	-0.35843664982825	-2.41488036748653	-2.43248561497308
H	0.56665141204328	-3.46427029891782	-4.08900874827047
H	-0.50143235645847	-3.49492488641833	-0.51949440191396
H	-0.23183107682658	-1.95633144777391	-4.55410061709596
C	-3.57744076049458	0.52437708278868	0.04290559604561
C	-3.22672020326729	1.98773786292837	-0.29429980694772
C	-5.10913205775801	0.42460510494082	0.03755119691876
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H	-5.54331484523600	1.09359714516846	0.78142881326766
H	-2.15540413143074	2.14680277096806	-0.36885311535213
H	-5.44080251935006	-0.59029152867942	0.25253320361004
H	-3.67461058585583	2.25870565073747	-1.25246654508137
H	-5.51341365822926	0.72417074275240	-0.92986256741356
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H	4.83060679321987	0.33466633459423	-0.33804505909605
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H	-1.18544049137026	-3.39784043546170	-4.17982413005555
H	0.41610385504321	-4.34142760266132	-1.75585587344040
H	2.34411955623967	-2.19027583913600	-3.61702922359909
Al	-0.43669338668959	-0.69298144584831	0.37999415979680
O	-0.46911169188521	2.10454718861067	1.31288875436419
C	-0.60405957580970	2.50070460754051	2.44739744792599
C	0.37621913904238	2.20129873303307	3.54207595139223
H	-0.13197876379933	1.64855758938895	4.33429131006861
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H	1.22159795471607	1.61327608248960	3.19460002822249
C	-1.81231790222293	3.31007074680934	2.84557769304612
H	-2.16781925042366	3.91831641158753	2.01626063366350
H	-1.62540847490730	3.93824988994724	3.71616969338601
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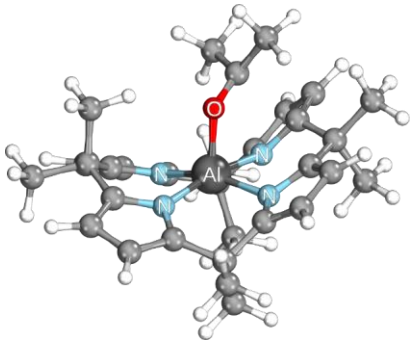

[**1**$^-$]-acetone TS 2

N	-0.11368780618160	-2.30337505064723	0.37503504439020
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C	0.32258027363620	-2.69988285120240	-0.86304216428563
C	-0.22168416100918	-4.54518191630543	0.26617567103851
H	-0.38732478462033	-5.57742216655901	0.53131840801032
C	0.26811905015285	-4.06853197086637	-0.96772322871316
H	0.55742583587359	-4.66394018106637	-1.82011358001060
N	-0.07198290929627	-1.11999375197481	2.83723116141212
C	0.47817872565521	-0.42043751247970	3.87896272622674
C	-0.37312542347270	-2.37474666639851	3.30826770799254
C	0.51463458960505	-1.20968434592758	5.00187430416322
C	-0.03336033091762	-2.45919089028221	4.63741600582935
H	-0.15364376111371	-3.31648793321865	5.28115936123999
N	-0.08510892595179	1.38039156416244	1.52667535385265
C	-0.79437346333312	2.40240742944773	0.93207062327436
C	0.20388986664495	1.79015026361469	2.79934160386282
C	-0.97110953573618	3.42583010369801	1.83259514136456
H	-1.46410862868918	4.36877767406867	1.64861977226044
C	-0.32433927688442	3.03684563382230	3.02867867622444
H	-0.25352144092581	3.61161703168034	3.93888947393699
N	-0.39602662387268	0.12731148435361	-0.86933235031200
C	-0.12560186598644	-0.56979764553186	-1.95839954059184
C	-1.32355649124978	1.11631804676996	-1.19015466799106
C	-0.86223536452332	-0.07237788402801	-3.05764390271087
H	-0.86796318637692	-0.47512761128807	-4.05847316008722
C	-1.60144910831608	0.98579397564764	-2.57461767726171
H	-2.25132924872113	1.62977551750013	-3.14959745571700
H	0.01676106463329	-2.81145445060079	-3.58612985001088
C	0.96484943657941	-2.38943609538112	-3.25150478181203
C	2.21821632102983	-1.18814327996338	-1.47399333359923
C	0.83175404062441	-1.72107344765330	-1.88585167443214
H	2.92793320091474	-2.01448600383710	-1.41339582835617
H	1.69542279350674	-3.19746627174706	-3.21131403830518
H	2.19376755851871	-0.70338662689283	-0.49834614687249
H	-2.82850974127243	-2.28541576545612	2.00748843349697
C	-2.54716968957913	-3.25126480759117	2.41648256720669
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C	-1.01558164584352	-3.44001189417656	2.45939757995941
H	0.30332157493152	-5.02726456075905	3.16546212197793
H	-3.00741610234282	-4.02972793488742	1.80266335183583
H	-1.24514543958483	-5.60071735106802	2.52961409707232
H	2.91940365219213	1.79810818619321	2.90380750201624
C	2.46675394086205	0.81515982065433	3.05465535177752
C	1.23628360266908	1.63386867383906	5.04743868155192
C	1.06764004831083	0.94945162448458	3.69236156854437
H	1.90759968053049	1.06117181141311	5.68831366981643
H	2.41954895028649	0.32126118852855	2.08376148955305
H	0.28055756689045	1.73507656984516	5.56171997659887
C	-1.03837561093088	2.47361066205835	-0.55153575504883
C	-2.10002071532910	3.51875628679128	-0.89791559099635
C	0.28437122762508	2.96969410181288	-1.19209263374469
H	-2.26171116512305	3.56747704260060	-1.97612732248408
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H	-3.05777958185736	3.33771426796246	-0.41893422101894
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H	-1.76319081905439	4.50768059278944	-0.58591205712904
H	0.55770474135134	3.93825513551000	-0.76971074493128
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H	-2.95906936799684	-3.31414240187175	3.42621215461299
H	1.66939829817141	2.62783818907022	4.92357118808638
H	3.12039356526002	0.21972180131934	3.69529187802712
H	0.90174364196066	-0.93527867342806	5.97097521272685
Al	-0.43545720648960	-0.48686140894168	1.05474545673841
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C	-2.92495449765018	-0.01923147593405	-0.07599463897857
C	-3.18753909090065	-1.13269834563966	-1.04547142901939
H	-2.28606526052041	-1.65877314078039	-1.35686604669824
H	-3.72856035587475	-0.79370038487857	-1.92530429276727
H	-3.80130181249792	-1.86833600008705	-0.51533956285743
C	-4.02448965657091	0.99434865565697	0.06647544875376
H	-3.72750374820430	1.79189904431858	0.74310810672937
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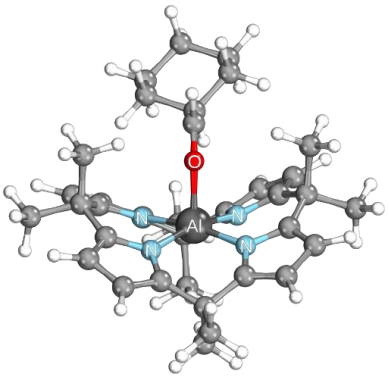

[**1**$^-$]-cyclohexanecarboxaldehyde sigma adduct isomer B

N	-0.13220252731327	-2.32569120776182	0.49436037293196
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C	0.27630308626560	-2.81539492959807	-0.71740162547482
C	-0.49159708786713	-4.54200112267720	0.46968868560545
H	-0.76086908225991	-5.54145824271901	0.77373037041980
C	0.05924055939670	-4.17132236586352	-0.77533654334609
H	0.29638190630829	-4.82955671036714	-1.59679195067023
N	0.00941792500835	-1.00759302037004	2.84312095092041
C	0.56713366040395	-0.25445833062929	3.84401923641631
C	-0.38965390166023	-2.19430648769178	3.41481672905845
C	0.50035325446041	-0.93107625354778	5.03576578908981
C	-0.11556671357983	-2.16968349220785	4.76173339130921
H	-0.31843926640437	-2.95212886957842	5.47623453584989
N	-0.06465865840847	1.42448095116466	1.48218998557858
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C	0.46121642692665	1.90806527351793	2.65058656510316
C	-0.39702503684764	3.64358359001010	1.54344994568236
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C	0.26556869814144	3.26454064962062	2.72876221001075
H	0.58193796102572	3.91797975751844	3.52660039468203
N	-0.14241146050835	0.12203219753942	-0.86277433683701
C	0.18503686976828	-0.67847416599788	-1.92201470514500
C	-0.78649371960912	1.22468870536077	-1.37156626053563
C	-0.27487772085581	-0.12300353256903	-3.09374484389187
H	-0.15105030671547	-0.51916372178150	-4.08991201720292
C	-0.90362805982061	1.08995671017540	-2.73949336805597
H	-1.34343693418079	1.80403754346448	-3.41972881592875
H	0.16466435488030	-2.96737990225362	-3.45816262474406
C	1.13083356504671	-2.67605648481389	-3.04348687387223
C	2.38376237104958	-1.58897951439080	-1.20250152610360
C	0.97267660348395	-1.93714574511911	-1.71715924413569
H	2.96800704110345	-2.49796485243772	-1.04638590545594
H	1.72883522713245	-3.57856975596474	-2.91204460164545
H	2.35299353850096	-1.05506613714531	-0.25231716571199
H	-2.96116902399471	-2.24363331638971	2.48175497083181
C	-2.58753996538635	-3.21732446212858	2.78189485459914
C	-0.66940487290162	-4.64782789110365	3.34995211778935
C	-1.05023892380207	-3.32297031113426	2.66671816819819
H	0.40559610107931	-4.81503459798897	3.31021114573330
H	-3.07788480759538	-3.98338357542250	2.17586743103186
H	-1.16856252264844	-5.49154457926635	2.87159846948711
H	3.16873207557047	1.65015914497072	2.65918866264140
C	2.62772196869644	0.72633923446853	2.87506142049252
C	1.57410367491428	1.77017760714116	4.86061994039869
C	1.27615351601078	1.03457356776208	3.55573320698996
H	2.19887995319768	1.15945420027170	5.51346525018525
H	2.49581345862658	0.19814535429441	1.92951609279033
H	0.65674963148363	2.01615217141646	5.39552836473011
C	-1.18865530730487	2.44880203200759	-0.57873370682580
C	-2.72079324940048	2.59235891388035	-0.47449813120007
C	-0.69274176763949	3.67755073612638	-1.36992609687802
H	-3.18745900140136	2.54596848756274	-1.46161145682569
H	-1.14453130452653	3.71393278298389	-2.36210374607998
H	-3.16756742894035	1.82611616587470	0.15465164311876
H	0.38895957009417	3.64631941417843	-1.48868667126905
H	-2.97498349744318	3.55293958126119	-0.02268280511931
H	-0.95456358217007	4.60578271248036	-0.86130016961091
H	2.90690533218572	-0.95079025066316	-1.91777529179174
H	1.63964966669380	-2.04639297104783	-3.77470689783251
H	-0.98091585797919	-4.64915728750119	4.39447362187416
H	-2.88904714701636	-3.35661775322401	3.82207202941320
H	2.11661755028590	2.69592463208284	4.66454850156858
H	3.24515445910225	0.09508363973370	3.51759903673645
H	0.86932041849870	-0.59340974201315	5.99148772605807
Al	-0.29745036682599	-0.44194342465268	1.01071770868106
O	-2.27016537232453	-0.44667902704954	1.02175040960291
C	-3.16651776534059	-0.79013858736408	0.27031207217231
H	-4.19375650327875	-0.68995619960293	0.66015476556431
C	-3.06978075576010	-1.36095199530028	-1.09080105815813
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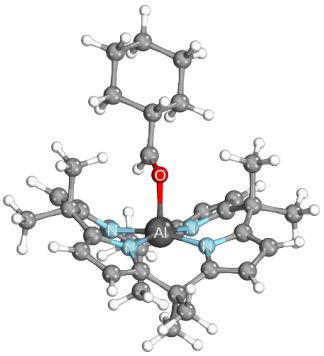
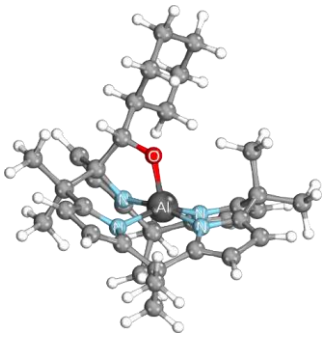
C	-4.03305578203316	-1.29781867631349	-3.40633924621801
C	-4.29890159096756	-2.79779888043111	-3.35007198448676
C	-4.07317894532990	-0.66694446271830	-2.01992547295358
C	-3.38215473243495	-2.86847982701167	-0.99605077210563
H	-2.31552308753335	-3.41886479263480	-2.76032802153228
H	-3.04624465753990	-1.11170906486167	-3.84001100088687
H	-5.33152513988966	-2.97290497996470	-3.02570393695418
H	-5.08653316490349	-0.74942911936622	-1.60501027546681
H	-4.37408300662344	-3.01901918808643	-0.55048178860070
H	-2.06224134198453	-1.24364264251433	-1.48983826283442
H	-3.57081419512016	-4.55415920945621	-2.31260696088826
H	-4.76134018544011	-0.80446785682448	-4.05523242238431
H	-4.21149994609595	-3.23378096556414	-4.34878476393261
H	-3.83420705382601	0.39444920416834	-2.09270077351804
H	-2.65229621867182	-3.36410376173251	-0.35499361232105



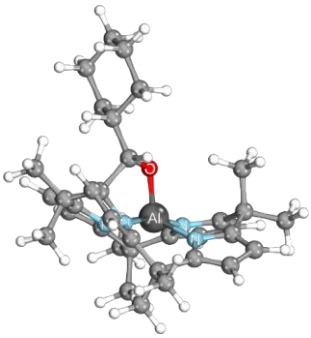
[**1**$^-$]-cyclohexanecarboxaldehyde sigma adduct isomer A

N	-0.43734374459476	-1.94571507797688	0.61258442125989
C	-1.24870756594720	-2.80296845952259	1.31669665705878
C	-0.50283402425554	-2.31677078796355	-0.70220140106882
C	-1.85731500032318	-3.67633937900593	0.43819290627645
H	-2.52839757369131	-4.48199908651273	0.69694364685249
C	-1.37237673378620	-3.37256070475956	-0.85324415037648
H	-1.61320255068386	-3.88527037571476	-1.77171651865562
N	0.28285307006557	-0.90860877248786	2.98433838495962
C	1.17048722863318	-0.44174511116147	3.91841763276786
C	-0.30734404045321	-2.02893257147993	3.51660038603144
C	1.12668021489860	-1.23174563799141	5.04035424054457
C	0.17859514430545	-2.24434936484631	4.78482931271769
H	-0.10465593846962	-3.03839569412309	5.45843239379241
N	0.63654874023533	1.57855503039302	1.82329781450790
C	0.37060961989457	2.80799519234489	1.26964343641301
C	1.48200724973466	1.79031694552305	2.88180526705091
C	1.01424350339963	3.78410734701424	1.99306946727534
H	0.98810048618614	4.84691699857313	1.80933260198738
C	1.72842810035437	3.13321500335548	3.02099770173595
H	2.36540351941249	3.59976774275002	3.75605938969265
C	-0.14535205160764	-0.14099574383456	-1.72595513471886
C	-0.51642120511203	1.86353192980299	-0.87980568839710
H	-1.00327327176181	-2.13443873677300	-3.40026736863797
C	0.04861482048732	-2.18767974463976	-3.11742129968620
C	1.79559066031934	-1.68282177544054	-1.43360521190110
C	0.29049371769868	-1.57796023987017	-1.73974553721125
H	2.11534638766787	-2.72695838816667	-1.43263957352424
H	0.35208993817929	-3.23559460082165	-3.13073400054602
H	2.05029124161013	-1.26473080786764	-0.45976057705700
H	-2.93422877653632	-1.33840742424867	3.14673928966654
C	-2.76321218556799	-2.40074735923950	3.30583623875493
C	-1.20045089323669	-4.31596493029431	3.25266656960298
C	-1.36588494267036	-2.84531413650932	2.82499990577987
H	-0.22838639269609	-4.69991408645093	2.94736128361109
H	-3.54864364196058	-2.96248214048672	2.79294944218264
H	-1.97159018464579	-4.94208927525211	2.80227257065714
H	3.99286581838639	0.84869276699122	2.44923365320106
C	3.26111651832874	0.07630991827227	2.69532605068061
C	2.80476430921480	1.15500377029952	4.88040843750895
C	2.14594770744924	0.65149673114050	3.59721939875401
H	3.32485256272705	0.34361427192493	5.39094175169556
H	2.86467461994469	-0.30744280597823	1.75363626801074
H	2.06755681955215	1.57498382328258	5.56459285834945
C	-0.53382208658657	3.02890833035898	0.08610709803307
C	-1.96162422871609	3.35991282468827	0.57243346125097
C	-0.03958554280270	4.27097523830970	-0.67641107565272
H	-2.63198965883606	3.51889645338573	-0.27672491770419
H	-0.68992032319067	4.49272527879602	-1.52326739676757
H	-2.37752629084749	2.57669979315801	1.20092961175394
H	0.97167595209234	4.12148723960096	-1.05111157902432
H	-1.94572920079275	4.27405397084321	1.16927965676973
H	-0.04322551470592	5.15226339666363	-0.03412813952595
H	2.37446226803679	-1.13865045873374	-2.18238923975792
H	0.62899852004062	-1.66088334591199	-3.87613081321233
H	-1.28919381237881	-4.42437384173496	4.33429892354021
H	-2.85985202601838	-2.58047674231447	4.37820017389121
H	3.54531442439406	1.92421228684128	4.65803281803717
H	3.77032616461024	-0.75071905254046	3.19468886941209
H	1.71996409159849	-1.11749675353060	5.93400686656932
Al	-0.09761416166360	-0.11604084190329	1.26366401603766
C	-2.79322042115778	-0.24081397882815	0.50633578055719
O	-2.06280509919388	0.20780881973500	1.38081685841053
C	-0.85180442125757	1.91790984304366	-2.21591090201220
H	-1.18927976705155	2.78749896541524	-2.75930752031331
C	-0.60929489050615	0.63699168606152	-2.75934311957986
H	-0.73265650176373	0.33791010491958	-3.78887153100538
N	-0.10451609757830	0.58842037964769	-0.56950604922505
H	-2.39040713769640	-0.88939402785813	-0.28454995740311
C	-4.23817974721353	0.07781220358109	0.39885424726080
C	-5.92945512730148	1.06635801677101	-1.19291142172975
C	-6.53104732397467	-0.95209352230461	0.17552162906158
C	-6.74388735266273	-0.22099219747708	-1.14490029970289
C	-5.05437608797247	-1.22307263178363	0.43822844954309
C	-4.44990805822741	0.80302742370424	-0.94289165622594
H	-6.30713858328669	1.76552745326499	-0.43905245380237
H	-6.94069383041416	-0.35033290913107	0.99408061346233
H	-6.43941407384708	-0.87164096557272	-1.97159110868751
H	-4.66046202106626	-1.91752379100134	-0.31121560085159
H	-4.03776686416283	0.19124586176562	-1.75216717203577
H	-4.53303948893956	0.73172689199358	1.22577774666146
H	-6.05179991720563	1.55992266720091	-2.15972176348173
H	-7.08149338055955	-1.89582071156203	0.18234718346997
H	-7.80527007523946	-0.00628216085875	-1.29318380806744
H	-4.92360103087198	-1.71314422602925	1.40393540534003
H	-3.88291855576819	1.73447277707834	-0.95685461888881



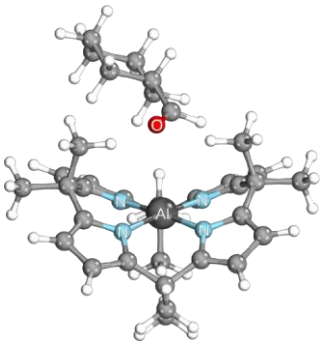
[**1**$^-$]-cyclohexanecarboxaldehyde 1,2 adduct isomer B

Al	3.46787891571615	8.90754006210306	2.74563765363644
O	3.35116693979091	8.36804980809328	4.44611482897480
N	2.98072061108705	10.74300324605711	2.55441217439114
N	5.39433030188077	9.25892516481875	2.71061138371551
N	1.83678942618398	8.40270249044346	1.75866979541590
N	3.96888225660983	6.98668311186099	2.43165621865061
C	5.90696965422768	10.52484107861300	2.75344322310956
C	3.80280159238704	11.81786441005776	2.35493913281977
C	3.88701174881949	7.16468003937027	4.82406746598084
H	4.66446003954997	7.31824167804925	5.59076738987851
C	0.64920262644627	9.06101838839169	1.92233869523173
C	0.25614065539450	7.27425991087621	0.62727031009251
H	-0.23434413411009	6.54129000186109	0.00460150855292
C	7.06812547472393	10.53897279853118	3.49067801799852
H	7.69443544040374	11.39289912586151	3.69639422338029
C	3.04995386371131	12.96802124903410	2.31767868262848
H	3.41229174734348	13.97237384132713	2.15993668661606
C	1.69357087697715	11.21021998449915	2.61282122695650
C	2.82173608980013	6.26927615379896	5.49108991122519
H	3.27970488736534	5.28915783551049	5.69680554900791
C	2.68123990645060	6.37216235978931	0.50541914669532
C	-0.34644513909914	8.39306193879689	1.24066500832793
H	-1.38781628582362	8.66852591934183	1.18344464409777
C	5.25842795207957	11.65206346713768	1.99933942670032
C	3.51215708057062	6.03787968068144	1.70979799244024
C	1.58985996981632	7.31402853394470	0.96522437470150
C	1.56158214693018	6.04984340281788	4.65299146075973
H	1.12801820047372	7.01643948782944	4.38885886274096
H	1.79548275518291	5.56122664658018	3.70817325266614
C	0.51154446130318	10.29091086599893	2.79346735624228
C	6.24449106223385	8.45696205477756	3.43960723423225
C	4.50864424581452	5.00768399388801	3.44031710712503
H	4.90408362628918	4.27637003483849	4.12998762163699
C	-0.76684943790686	11.03636702280076	2.40138918045593
H	-0.74348900919692	11.34763258698169	1.35728410337955
H	-1.64418113951986	10.40635992505415	2.55503282476749
H	-0.89663554485450	11.92329918665390	3.02279422183890
C	3.85421499314538	4.74497337344690	2.29901300278692
H	3.59120671253863	3.77759388189686	1.89886974691216
C	1.70095713716528	12.57938606014085	2.48511996228420
H	0.84308453474184	13.23385406748569	2.49576384686920
C	4.64258272505575	6.48603642535007	3.59360230987606
C	3.58665732375359	7.05095922867203	-0.53959687423473
H	4.03593213818351	7.96435975729833	-0.15137721106641
H	4.39638823007689	6.38942122354448	-0.85996065727416
H	2.99194814554931	7.31859261293796	-1.41340021885286
C	7.27969485878308	9.21559833819237	3.93543632481786
H	8.11020808871401	8.86889423970942	4.53189616983430
C	6.00911798805401	12.95456780511681	2.27186805128921
H	5.95790456577320	13.22702653213519	3.32600931484665
H	7.05902680048821	12.86187312541956	1.98850111783172
H	5.58545858056630	13.77297930948398	1.68902306533435
C	2.44114047571672	6.88101666455941	6.84349192897200
H	3.33808256810469	6.99600875780277	7.46058075907170
H	2.05228027779269	7.88943574231763	6.67639992582273
C	6.14419676114942	6.95099489783462	3.49119958824902
C	0.36228105688940	9.88864808436968	4.27602329953067
H	-0.49108293096031	9.21697620062238	4.40385265081247
H	1.24825678714518	9.38714383812722	4.65853283501349
H	0.19767932309206	10.77930849432116	4.88675611418445
C	1.40331295168833	6.04831335559711	7.58746535484723
H	1.83337934031091	5.07319197337309	7.84711526630857
H	1.14221839930900	6.53095692860592	8.53368777437800
C	5.35864826564168	11.35339326315713	0.48763458728506
H	6.40116243315526	11.22429198190002	0.18619371576017
H	4.82112984145246	10.44069282663141	0.22923718774049
H	4.92084505568492	12.16883912945537	-0.09153528013094
C	2.08654206491294	5.10728528088418	-0.10738290087470
H	2.87261728495426	4.42002021278326	-0.42772210829580
H	1.43454144231228	4.58724418869536	0.59536890219470
H	1.49452858133140	5.35707273421654	-0.98719019114964
C	0.52232446650999	5.21437305530321	5.39501100979183
H	-0.36932351215958	5.10397535988781	4.77249412585291
H	0.91163319096072	4.20202972775236	5.56101495319428
C	0.15654876665024	5.83418203485324	6.73758619637336
H	-0.56702058324012	5.20786718944273	7.26804369233085
H	-0.33203974959907	6.79926383779529	6.56526791202510
C	6.93978070267488	6.39870153181638	4.67700537265216
H	7.99200525090666	6.66349509273087	4.57565314974193
H	6.59692740030287	6.79340279442117	5.63207470356624
H	6.89151668668927	5.30867115433830	4.71640320626994
C	6.78886255017900	6.39316951746924	2.20806775941870
H	6.28117141843391	6.74785385834118	1.31227872355293
H	7.81620231936616	6.75333712712151	2.15370023423184
H	6.81087542500040	5.30088269557065	2.18630170295425



[**1**$^-$]-cyclohexanecarboxaldehyde 1,2 adduct isomer A

N	-0.05555737930004	-2.29023605927228	0.41151480142696
C	-0.31303169709309	-3.46939298070224	1.05607916336275
C	0.37139303599711	-2.60777119232900	-0.85137047022573
C	-0.04692557288092	-4.52621376510372	0.21173606791554
H	-0.15773203689862	-5.57559976128845	0.43510280745636
C	0.39078173288841	-3.97433136093134	-1.01059242537651
H	0.68951305025924	-4.52088858773589	-1.89232121041940
N	0.05944160115891	-1.24151781594487	2.93383327681705
C	0.69139059545517	-0.60068590116527	3.96438292738529
C	-0.22829895995737	-2.51497024030302	3.35097190310286
C	0.77946024939384	-1.44803674317340	5.04341953322788
C	0.18928619385173	-2.67180778616686	4.65155905014341
H	0.09991750772646	-3.56121136380551	5.25590382275187
N	0.15170278898225	1.28651096453595	1.65909426505658
C	-0.48392410409439	2.37328521623679	1.10240698356549
C	0.56262847797985	1.66269280915359	2.90762886392632
C	-0.46912304095635	3.42216886709257	1.99272340437559
H	-0.87592092774957	4.41004882747934	1.83590070494662
C	0.20413244066653	2.96828001294260	3.14876341567558
H	0.39560022901385	3.53727854093297	4.04497151463604
C	-0.19581919297071	-0.45160953165088	-1.81146493787495
C	-1.51655459160790	1.07327839720570	-0.82813245254863
H	-0.05717468301341	-2.59375416066727	-3.57123052553862
C	0.89386756011254	-2.16187700616341	-3.25821420364840
C	2.18665611206388	-0.98814782487770	-1.47969791216910
C	0.80855774137934	-1.56573472412081	-1.85578123078423
H	2.92808308770917	-1.78737772204251	-1.49293978228373
H	1.64246812389885	-2.95282484737282	-3.28691703476570
H	2.18187244845846	-0.55587701222058	-0.47968757058678
H	-2.67598042066951	-2.31138626690628	2.00812961268777
C	-2.41957199459040	-3.29329340434338	2.39900735255898
C	-0.67450267895394	-4.92660654675887	3.02767036594323
C	-0.89429410458115	-3.52564594652822	2.45116018762326
H	0.38535517882758	-5.17330176791983	3.08706329145854
H	-2.89308101108503	-4.04468233485009	1.76207141528904
H	-1.17149340252074	-5.67903226091794	2.41362859372162
H	3.26035789583315	1.44294492807611	2.95026758868773
C	2.73573761325901	0.49684373217985	3.10483526126059
C	1.61480510741577	1.38495297274088	5.13525979821022
C	1.36493230851738	0.73414682306698	3.77580753912678
H	2.24154703073897	0.74671699239085	5.75879123863926
H	2.62215113714430	0.01549456545072	2.13317231508776
H	0.67963976555890	1.56483071244334	5.66548218873119
C	-0.93047062473388	2.43994076118798	-0.33811153653530
C	-1.91628374065949	3.59182252674590	-0.55678321156311
C	0.31723606331486	2.78138829258183	-1.18469496787833
H	-2.24660542667873	3.63801370894371	-1.59635528494304
H	0.08941996379871	2.87946547316011	-2.24931305470001
H	-2.79449656824318	3.53601063493743	0.07915768756394
H	1.10724615255016	2.04253698659142	-1.06406970375791
H	-1.42305690076806	4.54043883525377	-0.34329572332138
H	0.71808338839949	3.73353764495243	-0.83690973037069
H	2.50221401730773	-0.20995804030181	-2.18028069037714
H	1.19162601045333	-1.40578346236145	-3.98806439868124
H	-1.10121931796529	-4.99778618529887	4.02885398568674
H	-2.84125405909536	-3.37359556918006	3.40364838482677
H	2.13479302867108	2.33714176442205	5.01741357066461
H	3.35544088674252	-0.15449321628181	3.72435908226924
H	1.23758643169229	-1.23421170196173	5.99690582966829
Al	-0.43090125568369	-0.53436529104060	1.23209989663675
C	-2.68070558652172	0.33054053114365	-0.01235505318215
O	-2.18953715564986	-0.20324023012229	1.14636451149166
C	-1.80755649114434	1.04096257723195	-2.29068897048876
H	-2.55339205750316	1.64838933583520	-2.78300644059700
C	-1.01877656549738	0.12487790582970	-2.87219652734808
H	-1.00334488919064	-0.16717006703233	-3.91125370573735
N	-0.46335401930159	0.10144095841584	-0.69118024740592
H	-2.95273875987596	-0.47584469595375	-0.72150171142815
C	-3.97194832770260	1.13883192048012	0.22346437857724
C	-6.50046661961852	0.99873020535663	0.25938156621332
C	-5.30455473141088	2.62128909356519	1.76318439082764
C	-6.53559264989052	1.73726247951020	1.59315100016598
C	-4.02066833821084	1.81588432941113	1.59355742230217
C	-5.19609550267148	0.22970069289617	0.07290149595307
H	-6.60562617627189	1.72582639858922	-0.55483936775163
H	-5.33603135229920	3.43369041692609	1.02599470604073
H	-6.56223016085607	1.00568810164351	2.40787593043531
H	-3.97065329191826	1.04309854126144	2.36366013625558
H	-5.12816962953909	-0.57948877353543	0.80799189558698
H	-4.05739854384921	1.90757221241426	-0.55742575152505
H	-7.35505560314591	0.32087835133668	0.17738975540729
H	-5.31810217786632	3.09992051759953	2.74593628106555
H	-7.45285426142359	2.32789866094868	1.67613124361308
H	-3.14255546850019	2.43984848029401	1.76517658229279
H	-5.18776690461076	-0.24732655306144	-0.91204885452888



[**1**$^{-}$]-cyclohexanecarboxaldehyde TS 1 adduct B/A

C	2.48307553906019	2.47307473920483	0.76314497062122
C	-2.77367362125904	3.14221943547310	2.19850981478591
C	-2.43905187245596	-0.20751869621915	-2.16206829020444
C	-2.34391717722990	3.77965008482463	0.85817022011454
H	-2.32350978403927	2.15845452564120	2.34760549461887
C	-3.99849909722846	1.82354404097583	-1.81654245134641
H	-4.76834959903633	1.57784594794744	-2.53105767539942
H	-3.85685450063691	3.00911940593162	2.23033082606573
H	-2.46582803893871	3.76819159693768	3.03843994908688
C	-1.44745995404847	0.12558863242027	-3.29556821444285
H	-1.96135548504677	0.69819774096606	-4.07063914020051
C	3.10671235077977	0.27215687093906	1.98353897928760
H	4.13792605372159	0.48860706956341	2.21497321880796
C	2.40062120993884	-0.90649045464028	2.32244332064072
H	2.78510433471475	-1.75448196725818	2.86795861002935
H	-1.04089777001323	-0.78459974852684	-3.74032858566544
H	-0.61104475266748	0.72505680677151	-2.94835693432921
C	0.35497076569629	-3.00542776938786	2.54762965174261
H	-0.50979670049699	-3.65787384533304	2.67520762071802
H	0.83273044683190	-2.89788181555208	3.52238396750315
H	1.05951977189401	-3.49997365160807	1.87908770728291
C	-3.64124118932898	-0.90197236202941	-2.80986367068989
H	-4.39698393629074	-1.16229403054237	-2.06966348419230
C	-3.02820115131181	5.14187693307924	0.75479806740050
H	-2.74017713863745	5.78315193534705	1.58858916246392
H	-4.11269041620487	5.03299322363791	0.79146323743510
H	-2.76445145470106	5.64605319725997	-0.17452606795840
H	-3.32989034274285	-1.81406292961445	-3.32078875038465
H	-4.09937466077662	-0.25782598737473	-3.56114293841232
C	3.66579994013959	3.09885943559399	1.50738039499322
H	3.88681572800703	4.09130958666456	1.11309278607288
H	4.56602852881558	2.49665522679648	1.37746868880991
H	3.46185356903857	3.18807324148423	2.57377618984326
C	2.86813710671922	2.41031861273279	-0.72875461290873
H	2.05482725146268	2.03943385173283	-1.34724612356756
H	3.72990977772645	1.75558041678122	-0.88060877226395
H	3.12347290045873	3.40980737191931	-1.08647202519483
Al	-0.52586604811237	1.09697314587155	0.25199883138792
O	1.26473524895313	-0.24646028523911	-1.77315412705389
N	1.00373782832932	0.47145186199267	1.23604375498425
N	-2.13279626087086	1.72900579621081	-0.57437541644287
N	-0.00294338178569	2.89062250336520	0.67772819044436
N	-1.12475733886956	-0.69742599028970	-0.04851557047831
C	-0.85331749054545	3.95550888105972	0.85712249927089
C	-2.88987353390782	1.07362842324380	-1.51779836727741
C	-0.77058627196421	-1.79743570856844	0.68635065866864
C	1.27104900952209	3.34704125958936	0.92341908099060
C	-0.07490261635947	-1.64320018936247	2.00937879162913
C	-2.79127611799494	2.89641930609590	-0.26956147942202
C	1.12048022928543	-0.74756605819789	1.84979991737590
C	-1.04819618852660	-1.02980185436244	3.03797421666918
H	-1.41155867071509	-0.04614406131156	2.73504623413744
H	-0.55623186277277	-0.90636813087466	4.00473742290030
H	-1.92397719840105	-1.66918166925397	3.16405331585351
C	-3.93840521854639	2.98691929882241	-1.01450219146884
H	-4.66672555253387	3.78205394935914	-0.98108388919920
C	2.22172488301947	1.09932647673017	1.32935800088991
C	-1.84248354071987	-1.13759106091670	-1.13373513207293
C	-0.13082751539374	5.07090181652995	1.19390643246716
H	-0.52431947424789	6.05141178509346	1.41164543005939
C	-1.92226203545450	-2.50983178934976	-1.09390708670962
H	-2.43146717216968	-3.14566340284287	-1.80134128409509
C	1.22862238564122	4.68293866258543	1.23025119682456
H	2.07015621109511	5.31869268454260	1.45669100279630
C	2.08197944812170	-1.01024068762549	-1.32361215389470
H	2.67400197620462	-0.74633625190958	-0.42948523824861
C	-1.24175384086950	-2.93238082376145	0.07358442284347
H	-1.14587581100470	-3.94604947016113	0.43240120981696
C	2.39126687473821	-2.35307060651451	-1.92550167619528
C	2.76768959812995	-4.78832132746613	-1.39119796231614
C	1.78601806891732	-4.12001420984388	-3.60836036297113
C	1.80753296122653	-5.17842474208501	-2.51033466581662
C	1.44173196365275	-2.74270847611102	-3.05074968036589
C	2.41918440930417	-3.41775919828343	-0.82389353842845
H	3.79357995510140	-4.77801931048964	-1.77841528168617
H	2.76761224521909	-4.08680207766518	-4.09650840977759
H	0.79971635431488	-5.28300683592641	-2.09526396353679
H	0.41967780109551	-2.74460530029993	-2.65844730840787
H	1.42939814450503	-3.45309988842157	-0.36007988714331
H	3.41700748097480	-2.26702167366132	-2.32229741086172
H	2.74579722878322	-5.53643113018204	-0.59443768348098
H	1.06718883241019	-4.39628930713242	-4.38399646208137
H	2.07992274715212	-6.15335981545042	-2.92425976387514
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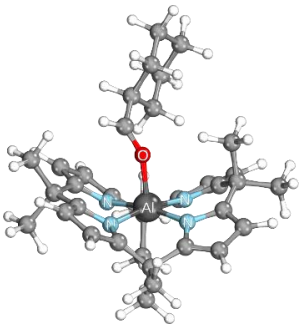
H	3.12150080819598	-3.12919641516867	-0.03737559378524



[**1**$^{-}$]-cyclohexanecarboxaldehyde TS 2 isomer B

Al	3.65723494086124	8.79115736680791	2.44128368693862
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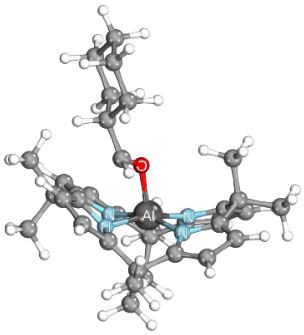
N	3.11662377458688	10.66050109634566	2.46139784870185
N	5.53500322269291	9.27432230499772	2.66792547048704
N	1.84311720488927	8.34032970933268	1.85016272457974
N	4.27912799193475	6.95587851120075	2.06037989346785
C	6.00844499202805	10.55646286898758	2.69841255409464
C	3.91569188799209	11.75327233058308	2.23449413086997
C	3.54528931536877	7.51834872976039	5.22779131088136
H	4.45640489640134	7.61475210576478	5.83822994733786
C	0.69761932478917	8.96603802964813	2.28598608191499
C	0.07830635708450	7.09840138353726	1.21146835420378
H	-0.51420606642392	6.31849158479153	0.75882492283093
C	7.13461223782248	10.62900570992731	3.48052334178562
H	7.72307826490103	11.50969552510649	3.68571040790241
C	3.17544290792271	12.90497596162513	2.31475203264072
H	3.53441915215092	13.91268373937943	2.17495449141501
C	1.84556190122165	11.14227029391424	2.68076862011752
C	2.55936120735734	6.48690451641343	5.64824314900174
H	3.15154627782718	5.59520628936849	5.89530775671121
C	2.44153482372330	6.30723473558576	0.52188760105190
C	-0.40045369706300	8.21944309645037	1.92158951546479
H	-1.43479436592006	8.45947021704208	2.11280574924394
C	5.36182893482624	11.61659730129655	1.86177238683739
C	3.50881273482008	5.96665097701118	1.51556051786210
C	1.44599906908120	7.21194648674663	1.18377821885661
C	1.52703943626153	6.14406760173718	4.58229626299463
H	1.00542566077544	7.04552002762415	4.24977870299556
H	2.03033647122190	5.73925132247653	3.70390998039037
C	0.66829886737522	10.27566396440899	3.03357396336014
C	6.40546307719359	8.51028731141592	3.41133616921817
C	4.96235533229992	4.98240213573018	2.89270936094213
H	5.55163474857593	4.23481561518850	3.40335023987003
C	-0.62304094983761	11.01703309402319	2.65640980742755
H	-0.66533610257583	11.21438603589562	1.58636065867399
H	-1.50133455864241	10.43343824973218	2.93385008539419
H	-0.69505498164678	11.96672462506929	3.18750092846859
C	3.88740021101086	4.73999692689396	2.00622724895462
H	3.45830046654166	3.78231849866430	1.75547000349890
C	1.85152768871584	12.51406111859147	2.60398753855790
H	1.00715728308966	13.17137985809070	2.73972521218803
C	5.19992126320826	6.34073229744557	2.87538523843663
C	3.06780358681919	7.00805619392113	-0.69892773897918
H	3.57743944979523	7.93246288888949	-0.42650741563757
H	3.80351104137506	6.36029314121006	-1.18066249097530
H	2.29457606318169	7.26400141118656	-1.42587956795290
C	7.38290817094924	9.31844046119361	3.94589319755638
H	8.22416106568557	8.99976640655130	4.54389678005569
C	6.08344683081948	12.94822386502553	2.05670541173529
H	6.01493976864706	13.28925726695044	3.08976767499345
H	7.13825744795516	12.85258493868214	1.79402545574804
H	5.65365109653470	13.71877160565514	1.41557337936255
C	1.89913376732260	6.98322019678718	6.95227623783712
H	2.65400588783799	7.17829990989320	7.71979640311839
H	1.39236064975329	7.93335877043218	6.75677631251021
C	6.47064096150192	7.00815039266926	3.33127634593656
C	0.60766956648618	10.05847560964762	4.56144406445423
H	-0.22593532484141	9.40120787949095	4.82346903757925
H	1.52169796426685	9.61798273804378	4.94703987710710
H	0.47088326109826	11.01513923530753	5.07005777599405
C	0.88246845568908	5.96496584137152	7.45807658650216
H	1.40487932569317	5.04799391966242	7.75259213347624
H	0.39919939395872	6.35054893304081	8.35947839140410
C	5.47960449777468	11.23268440299635	0.37194456839709
H	6.52694263795261	11.11854723588713	0.08331516675803
H	4.97701287684602	10.28973477189538	0.15328469933050
H	5.02189833866116	12.00061928165715	-0.25493380350676
C	1.75657723219269	5.03514426005063	0.03068293633782
H	2.48249107085877	4.36578414967075	-0.43368987204162
H	1.27257808377347	4.50022800477053	0.84849922723893
H	0.99607184354931	5.27121008771445	-0.71484930228928
C	0.51137589435235	5.14090819131862	5.11268742951340
H	-0.23636926777341	4.95450733625935	4.33966185145978
H	1.00333828239814	4.18106704392931	5.30930170396468
C	-0.15549298852707	5.63815912694235	6.38984775299717
H	-0.86359505714592	4.89710321926787	6.77021894752404
H	-0.73658398039009	6.53865284782940	6.16421370723755
C	6.95628778362298	6.41226606332372	4.65650580591530
H	7.92481664064118	6.82638626004442	4.93785568364611
H	6.26563559650507	6.61160730694507	5.47591079644234
H	7.07881591990408	5.33106595219725	4.58093724234571
C	7.53576849342166	6.67576006574353	2.25400119297743
H	7.22827556221720	7.08033607446220	1.29010852587278
H	8.49914510601976	7.11875740515822	2.51418791081686
H	7.65616081629702	5.59555530251385	2.14539682038063



[**1**$^-$]-cyclohexanecarboxaldehyde TS 2 isomer A

N	-0.19774256876048	-2.19507237370220	0.44363132055161
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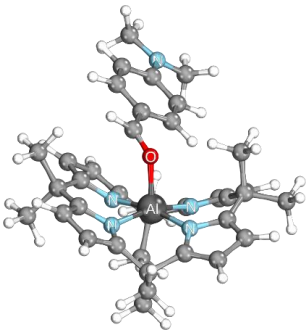
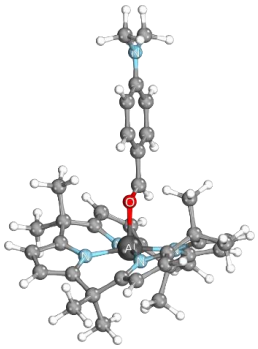
C	0.09468649991227	-2.58758493263042	-0.83720249461407
C	-0.52696559208674	-4.41207873797292	0.28486339980313
H	-0.76786656777321	-5.43310518494485	0.53531461685604
C	-0.09733033953106	-3.94032090051389	-0.97337488471170
H	0.06003724937372	-4.52950299532953	-1.86378615967917
N	0.22899965911983	-1.14599756536478	2.93317160321764
C	0.95915163836540	-0.56393774274125	3.93628427577204
C	-0.17659552766630	-2.37659702088870	3.38930268959236
C	1.00683416346180	-1.40229464577081	5.02216155694906
C	0.27792034379079	-2.56116894977033	4.67290766665356
H	0.11667427030701	-3.42678175749235	5.29623412023655
N	0.33576393563004	1.39915753449604	1.74596024862819
C	-0.31325293451749	2.51902719957309	1.27658580197582
C	0.82975850453318	1.71473002642324	2.98191648437800
C	-0.24747737457183	3.51697294590932	2.22069330388054
H	-0.64243881570287	4.51797509310144	2.12981738925581
C	0.49161140655485	3.00423393950938	3.31109239454616
H	0.74521429373275	3.52713498530974	4.21999320158291
C	-0.20348993674257	-0.37256744110057	-1.79834279905520
C	-1.11519187251380	1.39675446963365	-0.85289204471001
H	-0.48771398158142	-2.53654659059035	-3.51200161611624
C	0.53127502403583	-2.23703691658825	-3.26577655039274
C	2.08966663120770	-1.27844484973836	-1.58450717332097
C	0.61573748396620	-1.62547810461140	-1.86973428846373
H	2.69547273551352	-2.18463211358083	-1.62627468677019
H	1.16459024332164	-3.12164222274931	-3.33373194936407
H	2.22033312618402	-0.84059527128971	-0.59539004814632
H	-2.71482713042356	-1.93167803055168	2.33355169316974
C	-2.51566055598297	-2.94198665110022	2.67805428307102
C	-0.88518060650414	-4.73207733449558	3.13854844608080
C	-1.02146273980896	-3.31576607155508	2.56931999748010
H	0.14516787330886	-5.08306549752594	3.09228744228899
H	-3.12149840576952	-3.62958379739302	2.08267132945990
H	-1.51484265976947	-5.43230134865677	2.58804002938120
H	3.52410855214494	1.40959966795080	2.76866915646697
C	2.97766456833001	0.47792092220674	2.93306487362974
C	2.08266463045976	1.32704861712896	5.08536119785992
C	1.68407906125143	0.73716614181663	3.73415232297609
H	2.74471412602496	0.64726530979402	5.62299066252986
H	2.76642304613141	0.04410928585936	1.95504026001574
H	1.20848639330607	1.51379841820585	5.70911069186578
C	-0.76275684433551	2.69657723362108	-0.15189871152849
C	-1.90670780475609	3.70753175259274	-0.24115149926466
C	0.43868393075290	3.28560861586004	-0.93187346307559
H	-2.23959344492470	3.84158483559474	-1.27233890680198
H	0.18061101518416	3.47291566468168	-1.97767079967320
H	-2.76349710323431	3.41644942815699	0.36186394416336
H	1.28363075348285	2.59853515411057	-0.90618387195700
H	-1.57761248562568	4.68475585917043	0.11232907564009
H	0.75760985817857	4.22409663843104	-0.47534216669039
H	2.47643254422428	-0.56433591335407	-2.31575049877221
H	0.87609482062348	-1.52697293337151	-4.02001106900230
H	-1.21297242619750	-4.75960902660989	4.17822755991317
H	-2.83973184621437	-3.00440390572942	3.71935696426628
H	2.61807484490493	2.26826207160334	4.95007418731296
H	3.62325902096644	-0.22070453510849	3.46905621410945
H	1.51527385086286	-1.21978129348226	5.95622910698350
Al	-0.21591445349508	-0.39486440165994	1.22180202877873
C	-2.61397102143518	0.23717828489294	0.15540643829166
O	-2.04384834707241	-0.00261741783702	1.26786254390106
C	-1.58603485741725	1.33609412439842	-2.18716408580260
H	-2.25434336423812	2.04478436830376	-2.65447870749721
C	-1.04233196995964	0.21206329640465	-2.77241305464126
H	-1.23159881001769	-0.16686259353036	-3.76442267318174
N	-0.22919589176244	0.33310090798999	-0.67913887232868
H	-2.49178717768766	-0.48175593358696	-0.66827055260566
C	-3.96224522426985	0.92445181083399	0.18762734965763
C	-6.41802595082887	0.56759849188065	-0.26385112822254
C	-5.67406518992745	2.19224686023988	1.51106015520940
C	-6.75990926457582	1.21353314748733	1.07493049692001
C	-4.30681480729196	1.51877887459354	1.55030427526343
C	-5.03880222424368	-0.08410310414719	-0.23998893866915
H	-6.43805161396385	1.33182875569946	-1.04909266017979
H	-5.64699088642317	3.04014367927678	0.81633333812054
H	-6.86187515390358	0.43158128648557	1.83515462191976
H	-4.31523533478369	0.72236474092475	2.29966856795578
H	-5.03921949230554	-0.93011183113209	0.45610934328773
H	-3.95915035790433	1.72149064040715	-0.56258826913665
H	-7.17642342156428	-0.17194891465666	-0.53417806665504
H	-5.91378232615456	2.60797089765218	2.49278229124713
H	-7.72955052710685	1.71559408468987	1.01530550369986
H	-3.53467702199903	2.21783401702805	1.87668091255418
H	-4.79875126339522	-0.49184116599865	-1.22560384131495



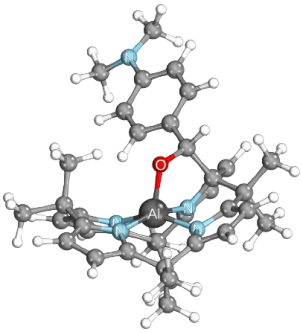
[**1**$^-$]-*p*-dimethylaminobenzaldehyde sigma adduct isomer B

Al	2.26771476900095	8.12628216822929	12.72896043232855
O	3.15827900376959	8.19869364869365	11.01759562197424
N	3.75526856187399	7.44027823268907	13.83350861858565
N	0.50740697005558	8.69588373519538	12.10158378180287
N	2.64280085272466	9.88906320880064	13.47103962898979
N	1.67968442719566	6.26768858359343	12.34209071683670
C	1.74231915718146	10.89481452968588	13.71466264272294
C	-0.08215893385970	8.19909084733290	10.96265884013380
C	4.23647741888120	6.21125495099556	10.24650189167255
C	2.29055607282437	5.13959016253001	12.79723938362609
C	3.87843807697459	10.37316048138127	13.83271751749888
C	2.88884030410022	5.11031305160766	14.17200519080865
C	-0.04429998675564	9.92858580282719	12.32396366233746
C	5.86846360406950	3.91787333096356	10.35827383401142
C	3.95032438183095	6.16229556085617	14.28601834675131
C	5.10365845980319	6.00264618961676	11.32359630030749
H	5.18276331520585	6.73155867305934	12.11619214157214
C	1.77970636953270	5.36925124767414	15.21145481433217
H	1.32057818032020	6.34832779698482	15.07602000145485
H	2.19293349781002	5.33528047991741	16.22157288177040
H	0.98837590576640	4.62086407344330	15.12936233173135
C	-0.93984044696677	10.23564470964494	11.32992501357496
H	-1.52677566928115	11.13684683361707	11.24488042779631
C	4.91746388406870	8.13322854759356	14.08811549790557
C	5.00551026035756	4.14097224516720	9.26127795265317
H	4.93284097759330	3.42321370539614	8.45735164117007
C	1.09215944570451	5.95082375303969	11.14070184294000
C	2.39024313044982	12.00235889732899	14.20043194073945
H	1.93897207118516	12.93930186902427	14.48752425078207
C	1.37861697564621	4.63385648482938	10.82728703282235
H	1.02715999397179	4.09053263912903	9.96203806704886
C	3.75893364115687	11.66930725938848	14.27283539481389
H	4.55512787893994	12.31019290134887	14.61760398863933
C	3.34466269281949	7.32554048186944	10.15696797072668
H	2.83789356890614	7.44876209736727	9.19127457825798
C	2.13981713682077	4.11240099615686	11.88654914469045
H	2.52944612524226	3.11015544446241	11.97239852206280
C	5.90792996493962	4.88757477136408	11.37368532096503
H	6.54484825403045	4.17605994357163	12.23840571092397
C	-0.01549680820281	6.76198625381799	10.51865261477348
C	0.26435363684197	10.68511951425808	13.57817982341304
C	4.21797168123334	5.26176665050756	9.21828174881585
H	3.53516546205663	5.39611384050534	8.38747296917864
C	-0.95638607369523	9.13043611377948	10.45206111723541
H	-1.58464854808848	9.01163857180223	9.58122384749293
C	5.83204648303423	7.29255997799260	14.68505194406711
H	6.82715486646704	7.55205539799672	15.01056642559962
C	5.21040765374674	6.03353807154049	14.81906692252029
H	5.63677849454110	5.14680302390803	15.26242206289160
C	-1.33676829603205	6.09430716960279	10.98108058334220
H	-1.40502293447335	6.12033104261886	12.06843047116007
H	-1.37984592280057	5.04979933219089	10.66419858794311
H	-2.20107335688012	6.62409971530984	10.57619669256609
C	5.14863064251042	9.57797701166875	13.72099310816745
C	-0.25184374473851	9.88362012339778	14.79232537873713
H	0.23198843907379	8.90922842173629	14.86847051365470
H	-1.32743438473627	9.71028661239353	14.71157979023195
H	-0.04910000857638	10.42379683712292	15.71947256984760
C	0.03091197110546	6.67927873304329	8.98751503876974
H	-0.86146670438340	7.12670786641982	8.54836166055105
H	0.07449905966641	5.64378840626418	8.64537107234866
H	0.88857720092191	7.21141920582900	8.57707820700748
C	3.48270356139939	3.73139139994990	14.45055966781799
H	2.71455957123189	2.96106090042250	14.36703883417922
H	3.89087951610579	3.68339355253820	15.46094215544647
H	4.28283584498927	3.49565105129243	13.74720322338559
C	-0.45866255675192	12.03027094978099	13.56917301105827
H	-0.27956588202033	12.57077934526720	14.49936877021090
H	-1.53613133806289	11.88490351481785	13.47634983239900
H	-0.12256200883433	12.65570881857072	12.74205075303320
C	6.18837813354929	10.16504171909780	14.68560537225837
H	6.39028395174056	11.20905051195187	14.44455447814014
H	7.13768421723645	9.63412405105497	14.60405535751742
H	5.84772986435560	10.10846938323590	15.71859559611149
C	5.75239223103312	9.70801478430908	12.30601798532585
H	5.06645143540178	9.37517384573393	11.53367354200224
H	6.67020072180053	9.11986836366112	12.22510087026231
H	5.99158367352513	10.75351634607518	12.09965853868920
N	6.63986117234948	2.79257891076989	10.42950063682045
C	7.37349930275394	2.51206996941962	11.63875729649355
H	7.90126465444264	1.56757659044099	11.53055072711295
H	6.72207730745140	2.43687887613314	12.51535215872920
H	8.12102691957508	3.28133645620859	11.84490228279224
C	6.49541378128008	1.75727965122462	9.44011267500304
H	5.49025106994999	1.32183006407466	9.42369774046825
H	7.20040068373855	0.95644595398554	9.64978464387781
H	6.71730533119431	2.12581709594103	8.43569952488933



[**1**$^-$]-*p*-dimethylaminobenzaldehyde sigma adduct isomer A

C	2.68848251736592	1.89249837536082	0.85809161672400
C	-2.43801706063989	3.42849590645412	1.89276939395397
C	2.30026440353993	-2.06618005671448	-4.23606030483447
H	2.50229035501181	-1.52711800511467	-5.14995106446481
C	-2.76343694066607	-1.16390914703930	-1.08719396144524
C	-2.01391924522432	3.56871997915381	0.41378610931440
C	1.75413101325235	-3.38929529914836	-1.86673180956408
H	1.52341236478196	-3.90269316349240	-0.94068756578775
H	-2.06838710916818	2.50170349709891	2.33443109063686
C	-3.95330960468071	1.06901886358399	-1.50194691775158
H	-4.76464069226783	0.69820466001508	-2.10974771799630
H	-3.52663140243540	3.42049977021406	1.98061292730968
H	-2.03904239058137	4.25367907066703	2.48661481643083
C	-2.16397435485279	-1.47798934000359	-2.47361194921880
H	-2.86722757026564	-1.18569651636050	-3.25594812942834
C	3.11496505171235	0.10199125127012	2.66024572757179
H	4.16032191752064	0.30263552022586	2.83615774464678
C	2.33081114911971	-0.86761555402027	3.32044757237235
H	2.65821825953569	-1.54586605165977	4.09338462774985
H	-1.95137692992286	-2.54417320159358	-2.58322721495130
H	-1.24497401225281	-0.92557091368584	-2.65396332000655
C	0.19467541839948	-2.72334885463340	4.05337171029161
H	-0.69874330484052	-3.29055582194167	4.31963873142910
H	0.66827727146496	-2.39394520100716	4.97908552972433
H	0.88650489889419	-3.39291699579218	3.54132927228535
C	-4.15570088711583	-1.82533714865956	-1.03961295479297
H	-4.63383201900436	-1.64479894515524	-0.07797790181904
C	-2.57735583690885	4.89089723431819	-0.10408341110571
H	-2.19465723694739	5.72817575011703	0.48091126505733
H	-3.66469605790504	4.90638968400122	-0.01927553783617
H	-2.31186380277764	5.05172291853250	-1.14894957005237
H	-4.07920946261629	-2.90385389420244	-1.18476433199933
H	-4.80622401620985	-1.43635391244318	-1.82413750992287
C	3.83065193196297	2.66726946512306	1.53392747195693
H	4.15699199762320	3.49988636900187	0.91010323105635
H	4.69986431765537	2.02541863211029	1.68337417824702
H	3.52154135170468	3.06051705526778	2.50113936786947
C	3.25745444385908	1.37946200719032	-0.48369596999815
H	2.49431596947198	0.92955923263957	-1.11050807760953
H	4.04198262844310	0.63876063343206	-0.31185116038937
H	3.68326734934508	2.21254197889839	-1.04766522095167
Al	-0.43595117573444	0.63821226778232	0.60896745075746
O	0.46955233430399	-0.18476088982697	-0.92047443015779
N	1.02650275926387	0.21712354396884	1.84523142666888
N	-2.09130077703987	1.15590125040093	-0.25262867753083
N	0.22627382299460	2.45391025953358	0.55233147885337
N	-1.32516103438054	-1.07883653867735	1.02747145927690
C	-0.51541433879553	3.58622084918575	0.33725236998587
C	-2.94411874162226	0.32431374845875	-0.93623652850021
C	1.44327329132637	-2.03519375050970	-1.98398322749059
C	-0.85818277383554	-1.98954696149765	1.93202828870038
C	1.54353129946033	2.84165774824880	0.61625652198601
C	-0.17259026630293	-1.52506753610588	3.18205787038420
C	-2.59052575658694	2.42574726173023	-0.36855466107865
C	2.62002691117258	-3.43690929205550	-4.12344964570998
C	1.06424803533140	-0.76356991733960	2.80013479840270
C	1.72330851300160	-1.38801909792367	-3.19019257626684
H	1.48310365741217	-0.33843579300206	-3.29977175910210
C	-1.12098057024765	-0.62302730705428	3.99461944176511
H	-1.42600898090238	0.26109306996193	3.43477194856233
H	-0.62665559840403	-0.27910517688323	4.90523118337094
H	-2.02941466971509	-1.16365930054993	4.26949812997866
C	-3.72986700747102	2.41255817112001	-1.13559582091568
H	-4.34726667453912	3.26003849729634	-1.38957757580352
C	2.28973353206853	0.75677033732390	1.77290133205118
C	2.32825317328180	-4.08411091749490	-2.90680564950991
H	2.54567302595255	-5.13324872922968	-2.77139316177826
C	-1.94932825567621	-1.78262563834238	0.02752971202972
C	0.31405113135949	4.67515789617392	0.23376419003737
H	0.01691305773451	5.70068321364628	0.07865048814407
C	-1.82589069049068	-3.13532791024961	0.27760693332080
H	-2.23769333259934	-3.93657622266384	-0.31860992396096
C	1.63100859652513	4.19799305579327	0.40774416095539
H	2.53153384120735	4.79208608555958	0.39511980186558
C	0.83290599667666	-1.36361508937867	-0.86676021555905
H	0.72989323255821	-1.94165416706083	0.06034818086775
C	-1.13654143765342	-3.26891659690610	1.50346841317215
H	-0.90551093733245	-4.18811380330146	2.01976608597067
N	3.19160835065685	-4.11139360942956	-5.16174704150763
C	3.50427957502297	-5.51046157710005	-5.02689228348078
H	4.21737398244590	-5.69742001748363	-4.21869238811109
H	3.95328919022922	-5.87179630082436	-5.94830801598683
H	2.61356564307460	-6.11602819560742	-4.83554919126125
C	3.47579467596693	-3.42962332987549	-6.39841569351607
H	3.93045304965331	-4.12559004096355	-7.09849763932304
H	4.17482783814001	-2.59987320300894	-6.26013643538534
H	2.57191582912765	-3.03290917784662	-6.86962490787263



[**1**$^-$]-*p*-dimethylaminobenzaldehyde 1,2 adduct isomer B

Al	2.06428190995192	8.03548609819738	12.53569611220494
O	3.09856797725366	7.98828630863338	11.07237499355034
N	3.75589636215292	7.42058983774646	13.44039370214213
N	0.26388298035805	8.51753849497204	12.12597496466481
N	2.55203672521575	9.81916758249025	13.16138708109743
N	1.44013328181266	6.20525046545658	12.94451288424954
C	1.71867249853545	10.89715692391661	13.05821719391734
C	-0.63516773196196	7.69325098673823	11.50073243970074
C	4.90225209383273	6.45551036132603	10.68938354630073
C	1.96559299295677	5.26553958635575	13.79199156893854
C	3.83451588000190	10.28294073752157	12.97658589506565
C	3.02937885865357	5.59331207678370	14.81523966751949
C	-0.37039771781125	9.70268382993491	12.38172143681163
C	5.84961931825142	3.91253198284090	9.85109927200926
C	4.09228705626480	6.38514011573523	14.11059633975289
C	4.12216381901528	5.31445067552133	10.82904537753880
H	3.13154720147122	5.37804281515443	11.25832805632512
C	2.44986404639308	6.45667879309114	15.95129877695275
H	2.01006947542252	7.37868305582180	15.57291899350816
H	3.21808053596262	6.72673036724911	16.68105686768700
H	1.66543816932040	5.89981567303215	16.46443916516846
C	-1.65537543945928	9.64755465745837	11.89585650037117
H	-2.40317918110285	10.42315782007097	11.95882263108013
C	4.87997553348423	7.96910099272746	12.73598254519642
C	6.62824762776595	5.06639718599513	9.69547930382786
H	7.61008911471342	5.01911422869174	9.24503823439750
C	0.47988783048331	5.58096553559917	12.19456675041570
C	2.45022048479588	12.03683450026949	12.81947059314426
H	2.06747533012834	13.03748086701175	12.69362163707846
C	0.40240666588272	4.25283087562141	12.55882892930268
H	-0.26013646421548	3.50810486215226	12.14659875091485
C	3.80467176733772	11.64146526140996	12.76060556652272
H	4.65183784063806	12.29077196148295	12.59784074867583
C	4.44507740497639	7.80756196483196	11.20058319131812
H	5.00330249462803	8.57311753336063	10.63901845687944
C	1.35332031202575	4.05110868379484	13.58219761388277
H	1.54829832118631	3.12721116646550	14.10531172542201
C	4.58537226873999	4.07152046953944	10.43398887157260
H	3.93091880582007	3.22555880645288	10.58968007809359
C	-0.28760486227782	6.28332496808004	11.09501098251525
C	0.23776993464718	10.75675869902753	13.27126699695638
C	6.15037238804700	6.30168272609297	10.10330552058593
H	6.78150916211084	7.17353602597940	9.95898671080663
C	-1.82395416385506	8.36266790642071	11.33044588867590
H	-2.71975931189718	7.98038196533974	10.86613476650305
C	6.00139908093692	7.07757787757872	13.15678354250323
H	7.02533507201762	7.17767496161838	12.82940222931538
C	5.52606414834810	6.14060980104289	13.98810244866041
H	6.07053377026495	5.32830233259565	14.44357604287895
C	-1.58020686151887	5.50915028344729	10.82149255432078
H	-2.21087013541592	5.45608110807970	11.70865437959499
H	-1.35901930906950	4.49282648440527	10.49250784605502
H	-2.14805681248927	5.98709138757397	10.02236319555980
C	5.07862937706006	9.45208079982736	13.18810142828281
C	-0.01267601569638	10.35716896636971	14.74185763869922
H	0.43632360449986	9.39026208318015	14.97070803049381
H	-1.08377307175403	10.27709937301671	14.93781751030124
H	0.41819645120733	11.09532449598986	15.42277923446199
C	0.52544182927868	6.27928347594163	9.78300374511819
H	-0.06120442227499	6.73930069862458	8.98461728911990
H	0.76726060096976	5.25460015283665	9.48925520732523
H	1.45833641739804	6.83142746616943	9.86659921395165
C	3.61663952895866	4.31883560600587	15.41523182374654
H	2.84208499084118	3.75403058351717	15.93308280006061
H	4.39403644634277	4.55203457960742	16.14592195623176
H	4.04377478505094	3.67396907328619	14.64661124115896
C	-0.44891251098458	12.09961397967182	13.02632271302846
H	-0.04207820677911	12.86743587536477	13.68663020354725
H	-1.51799865358942	12.02854798384978	13.22860772281317
H	-0.31997424124844	12.42688873352735	11.99466309698504
C	5.41645908848046	9.48643407926518	14.69170281748888
H	5.50692819149942	10.52572050001495	15.00749994174680
H	6.35554928727539	8.97732153611587	14.92240028720874
H	4.62457876954784	9.03787360710960	15.29058948706099
C	6.26148148739168	10.06738862983157	12.43457231147582
H	6.06146571775261	10.17955320884611	11.37025427462411
H	7.16892748206283	9.47219053000175	12.55656725556381
H	6.48038706593032	11.05959984026673	12.82851777891287
N	6.30303332883625	2.66784697939876	9.42826424846297
C	5.59062098536287	1.49764424386881	9.86719842836722
H	6.05825827783827	0.61092182483260	9.44214555539781
H	4.55791429961780	1.51049732423478	9.51536878363731
H	5.56695530523050	1.37858265316640	10.95862857673190
C	7.70144380354374	2.51446606482999	9.13645704752345
H	8.00621917619786	3.15663440181300	8.30749601516807
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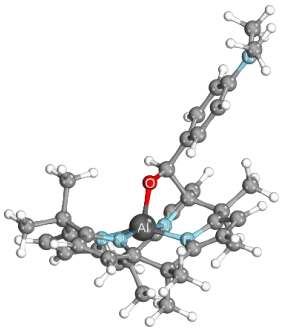
H	8.35811491009674	2.73877415553965	9.98848037445194



[**1**$^-$]-*p*-dimethylaminobenzaldehyde 1,2 adduct isomer A

N	-0.02595121846497	-2.32852685977424	0.40717409359662
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C	0.41166520208561	-2.62333909096500	-0.85811690742795
C	0.11004652059848	-4.56096639462138	0.20942941301980
H	0.06000906640636	-5.61454933277229	0.43450982991508
C	0.50919990725911	-3.98646414526545	-1.01569503622831
H	0.83325549851899	-4.51620694450909	-1.89869992457609
N	0.04955890578709	-1.27451901431384	2.93128627922971
C	0.65295371983573	-0.60301446902979	3.96001995069761
C	-0.16012150392167	-2.56422563477240	3.34649687170467
C	0.80141698347919	-1.44814761830340	5.03371347327789
C	0.27906133548739	-2.70241102609586	4.64178695198842
H	0.24621539381779	-3.59795317737187	5.24278516208735
N	0.00311092225939	1.26091510148458	1.65594864891881
C	-0.73485814577315	2.29260858056964	1.11686843210396
C	0.35432043813380	1.64485598046746	2.92064332341540
C	-0.84830975801245	3.30910163292804	2.03550797602291
H	-1.36038392677294	4.24921764729190	1.89730777835742
C	-0.14617639852246	2.89706063357417	3.19075304154990
H	-0.02641772602377	3.45816441071373	4.10440577169346
C	-0.28227348498326	-0.50393773681758	-1.81691022158090
C	-1.66815267750812	0.95506812630289	-0.82791806522053
H	-0.04295895016410	-2.63575100500593	-3.57543547594638
C	0.88660249426145	-2.15410239233430	-3.27042726172867
C	2.12843759966383	-0.90717193699229	-1.50543991847055
C	0.78099410501952	-1.56110455970412	-1.86796419006637
H	2.91325437749772	-1.66370249935876	-1.52670072700471
H	1.67569235732159	-2.90450018361157	-3.30479675210500
H	2.10925267803041	-0.47647323402949	-0.50487663665106
H	-2.62436875010304	-2.48161671705048	2.02279283507637
C	-2.31532114816806	-3.44976888769900	2.40960887601955
C	-0.48747084079550	-4.99542404073948	3.02527054503797
C	-0.78047429701018	-3.60694657963370	2.45156902046445
H	0.58370418017312	-5.18925966855755	3.07780367779353
H	-2.75578931054488	-4.22264641512315	1.77477472173193
H	-0.95030122438197	-5.77105024989976	2.41346970344523
H	3.06423017059142	1.62838069109692	2.94980459815490
C	2.61159202159570	0.64517510922664	3.10038123787396
C	1.43741745590218	1.43537966632914	5.14100194421902
C	1.23061810349706	0.77638517482550	3.77816398383723
H	2.11691001288250	0.84440021768185	5.75594664452632
H	2.52999076504588	0.16299082149805	2.12603382260063
H	0.49467670192144	1.53605811736725	5.67886814439752
C	-1.15218038941351	2.34834112832972	-0.33108294987232
C	-2.18188962099339	3.45837300561005	-0.56544632180160
C	0.09645579176823	2.73875043385534	-1.15306197425179
H	-2.50030355034387	3.48815359593084	-1.60903403394854
H	-0.11552308124447	2.82246915951602	-2.22225755407924
H	-3.06705216910371	3.36987269494890	0.05604954092843
H	0.91665538268437	2.03703654736352	-1.01373525326666
H	-1.72305255876226	4.42408014647847	-0.34964213447526
H	0.44678224697264	3.70985720578552	-0.80288845315316
H	2.39252188162487	-0.11210313856107	-2.20826687381419
H	1.13835513871758	-1.38425608930255	-4.00328414251665
H	-0.90378802494849	-5.08860096219706	4.02903450557814
H	-2.72616815670069	-3.55170174461422	3.41670585933477
H	1.87846195612979	2.42706300678733	5.02643983478865
H	3.28042748456147	0.03809410971962	3.71376937741295
H	1.25482569615559	-1.21085376203841	5.98393565117875
Al	-0.48108200619740	-0.59169804893904	1.22908882380501
C	-2.79816706732433	0.19390888328934	0.03068933322768
O	-2.25532869119800	-0.33347171207232	1.16449813033716
C	-1.96320468518051	0.91265309177142	-2.28734951318154
H	-2.73166346285070	1.49474702016911	-2.77452304298681
C	-1.13316849207345	0.03639608408083	-2.87379835034424
H	-1.10257136729472	-0.24690144616361	-3.91491331938209
N	-0.57549559186915	0.03105561967608	-0.69372080687761
H	-3.13126938126109	-0.60287622406643	-0.66081959397352
C	-3.99859999210254	1.05535710402892	0.32721817587331
C	-6.21980171663415	2.73446803511708	0.86472149391099
C	-4.17284804527146	1.63451627369654	1.57772150505363
C	-4.97241706401162	1.29491819515626	-0.63023219023658
C	-6.06131055818361	2.11515091050545	-0.38194949211385
C	-5.25496113668948	2.45514695334544	1.84333507820870
H	-3.43879424308189	1.45011145362796	2.35015508111083
H	-4.89287036001360	0.82210993297213	-1.60405263816235
H	-6.78867701046056	2.25472377920505	-1.16942882227809
H	-5.33489627134753	2.87747306117193	2.83503404839312
N	-7.28694329836796	3.58632612083707	1.12045299817566
C	-8.39312817750575	3.59288179917587	0.20314052742402
H	-8.07857954974302	3.90876465875888	-0.79380117880396
H	-9.13748800074528	4.31244732749301	0.54016563926586
H	-8.88862238941656	2.61758458353829	0.10187603447274
C	-7.55790931764027	3.95573382131608	2.48403853200757
H	-6.71432746580187	4.49160872721145	2.92249935598060
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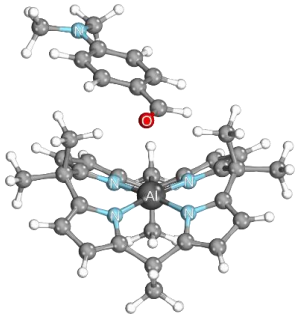

[**1**$^-$]-*p*-dimethylaminobenzaldehyde TS 1/2

C	2.51292877795582	2.57203263186249	0.81514528907096
C	-2.65959658893969	2.78846843160384	2.57292222847693
C	1.24529721570657	-4.02007885855610	-2.96305382922230
H	0.54185089063022	-4.40863528288889	-3.68498376702752
C	-2.50990343179044	-0.42735139155603	-1.85634889679325
C	-2.38125415007152	3.50929041454911	1.23459362563373
C	2.96405079591308	-2.96323069595988	-1.07620044538022
H	3.60981204518515	-2.55048732400256	-0.30927136221149
H	-2.12732312206652	1.83765110522376	2.64384264888208
C	-4.09877067318500	1.54144390822012	-1.38131953808193
H	-4.90488678406868	1.26939102340972	-2.04432458131607
H	-3.72441120426077	2.57091531533116	2.67782724211789
H	-2.33580812208024	3.40327712022444	3.41515520288643
C	-1.72178346466321	-0.07336184748938	-3.13395430152588
H	-2.35627639707964	0.50811514128335	-3.80600138198373
C	3.37396590443905	0.36732220309094	1.84976776617012
H	4.40313374775746	0.65058827069495	2.00595919525663
C	2.78974333107609	-0.87883774162781	2.17217915779666
H	3.28160553734159	-1.72212402975793	2.63196731969928
H	-1.40928300035718	-0.98052645650344	-3.65825201648959
H	-0.83376094295832	0.51274629736259	-2.92168423987428
C	0.96413588196986	-3.14883456250974	2.41629103569811
H	0.17312906565842	-3.87895739338136	2.59231854695067
H	1.54106410376761	-3.06153661204588	3.33810615526160
H	1.61733696983847	-3.53720056888380	1.63402919587664
C	-3.76042857095802	-1.19304607607452	-2.31029099007859
H	-4.38601930432556	-1.46819639692135	-1.46228421140447
C	-3.16865408954209	4.81829346336735	1.24414897338260
H	-2.86459593863122	5.44507657009812	2.08321774082287
H	-4.23621041452453	4.62524267072961	1.35555481659333
H	-3.01449137485859	5.37861512539928	0.32225952338778
H	-3.48425547302059	-2.10324227880849	-2.84394651305523
H	-4.35477407991030	-0.59162940621967	-2.99909860721006
C	3.66403135776773	3.25378493527410	1.56332869611675
H	3.79737165422637	4.27826558222604	1.21431330582857
H	4.60506966119091	2.73311707762060	1.38164406748699
H	3.48303664024300	3.27483991314432	2.63728689602885
C	2.87096789745392	2.60673906481394	-0.68486721264973
H	2.07696649300409	2.19922017644334	-1.30428717867250
H	3.78059805569543	2.03276197143620	-0.87973384831412
H	3.03932364735725	3.63874743204589	-0.99947050823921
Al	-0.42997008527516	0.97700053563972	0.40330207466420
O	1.13369583026124	0.05388057438865	-1.72041463211532
N	1.20151921742821	0.44460231040893	1.29688821783814
N	-2.14826944393522	1.51601948158883	-0.26998375265379
N	-0.00426310091218	2.79787801246941	0.86499482494505
N	-0.94801171319487	-0.85109170382616	0.11664069097264
C	-0.91356132785080	3.79409309971896	1.13100744362683
C	-2.93812908796262	0.84011450116756	-1.17170659341680
C	2.04609364396559	-2.12882160175027	-1.70523234829739
C	-0.43505127218457	-1.94653211975781	0.76206200728647
C	1.24600685059708	3.34345496946635	1.04630638464860
C	0.36770644105102	-1.79951701945196	2.02249467178754
C	-2.84569891164270	2.63933492304732	0.10626331630984
C	2.16993645077014	-4.87177678424941	-2.33014117220300
C	1.46409327600662	-0.79441461304670	1.82039476632948
C	1.18507042526106	-2.68161082734150	-2.64984428620324
H	0.44345483555566	-2.05160924448738	-3.12042584737563
C	-0.54976692827008	-1.33673709620401	3.17297585680314
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H	0.01915261617511	-1.22826022306202	4.09870638199215
H	-1.35446939972449	-2.05691798179816	3.33317998859358
C	-4.04211122003256	2.68936780403285	-0.56015565373265
H	-4.80543098810366	3.44462865413247	-0.45746091217424
C	2.37669710675154	1.15872915732914	1.32549821379831
C	3.03181317081137	-4.30853909348060	-1.37236627863422
H	3.74523681268053	-4.92014508219688	-0.83933861772203
C	-1.72568706481301	-1.31541974846888	-0.91936882204510
C	-0.25503018048821	4.95290054492548	1.45024116256160
H	-0.70477368825676	5.89530566788343	1.72078163393497
C	-1.68259118580678	-2.69073208673370	-0.93209158897601
H	-2.19159426088417	-3.34345023902668	-1.62414451292522
C	1.12701778678466	4.66562253621405	1.39128858866773
H	1.93315757378634	5.35542989718774	1.58552523737774
C	1.96204503820693	-0.73149569194077	-1.30089459161755
H	2.72093826035007	-0.41232735482482	-0.56790296211024
C	-0.86397549813605	-3.09391734808843	0.14465352227783
H	-0.62573412623365	-4.10720763255223	0.42759478223541
N	2.22515275735022	-6.21102349166767	-2.63654622122474
C	1.18464782159404	-6.79272059511864	-3.44433562084483
H	1.38568491902164	-7.85280365235499	-3.58264276942731
H	1.15123061097464	-6.34163167581676	-4.43833697109071
H	0.18852704707118	-6.69359322841903	-2.99809661231032
C	3.03788857862015	-7.08461559210237	-1.83233536035958
H	4.09032827310406	-6.79464619288990	-1.86758830876617
H	2.97416686090459	-8.09802725758642	-2.22257186160010
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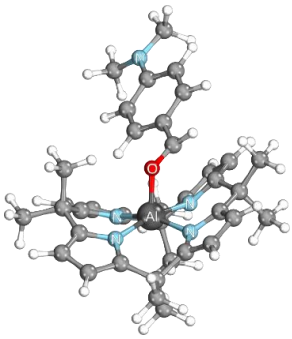

[**1**$^-$]-*p*-dimethylaminobenzaldehyde TS 2 isomer B

Al	2.08431435472135	8.05532414418930	12.61234299069499
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N	0.25643793489021	8.54371960853230	12.23011573632784
N	2.57076054366917	9.88298509190379	13.10024192890141
N	1.47797984613264	6.19154100385128	12.84135270991804
C	1.70383180880757	10.94065593057355	13.06851369607176
C	-0.65584578902266	7.75740138282736	11.56986056825494
C	4.71055966011532	6.39365413609927	10.59888081433891
C	2.05178116818432	5.18117970003174	13.56673184937953
C	3.82371528056527	10.38879218856007	12.83731257515839
C	3.16385351803227	5.42843128653356	14.54644126468283
C	-0.37956300157846	9.71658703503902	12.54385545894445
C	5.76417776444483	3.80558018469613	10.15694429256993
C	4.18989434063773	6.31778727254736	13.90884393662646
C	3.94067303426193	5.25721818157395	10.82946464807074
H	2.91673678446423	5.34358602172679	11.16055360913462
C	2.61878374180114	6.13098402633746	15.80594605110627
H	2.13167236296595	7.07472820596887	15.56251518351150
H	3.42068682811639	6.34524033913893	16.51653760201382
H	1.87986292288691	5.49362756398972	16.29412405177888
C	-1.66886440144487	9.68869398528689	12.07308878409631
H	-2.41051975605322	10.46536131218775	12.17804126561454
C	4.97063660882090	8.12148211392458	12.91744267653714
C	6.53708323491235	4.95970629342425	9.91241256335261
H	7.55423565091442	4.88049794809931	9.55564176392837
C	0.50624472312459	5.61625117779443	12.05695544594296
C	2.37885263964297	12.09911231242037	12.77160978414600
H	1.95710558802394	13.08784979706307	12.68053925729544
C	0.47667914195292	4.25763909372361	12.28412128354431
H	-0.18354624341345	3.54172318266400	11.82042015539204
C	3.73695388175940	11.74346859239015	12.61670906402222
H	4.55566157448790	12.41734980121118	12.41182697644585
C	4.21705693978517	7.74164291379527	10.84509436886398
H	4.84894388395789	8.54431437186087	10.45137314129650
C	1.46321612287573	3.97942372084926	13.25378931670626
H	1.70024385666653	3.01407566076501	13.67400738665122
C	4.45683459577902	3.99056864885632	10.62030548762830
H	3.81073926911239	3.15228168976169	10.83708196790051
C	-0.33348051085578	6.37928350208675	11.06018849647056
C	0.25877403057488	10.75536486821516	13.42113295092103
C	6.01343974075419	6.21150773203527	10.13289288550983
H	6.63950749405488	7.08017041806825	9.95859954961258
C	-1.84475782329064	8.43556410553554	11.44672447625396
H	-2.74510795920793	8.07919816829146	10.97120715582394
C	6.06130953742119	7.24533594862815	13.13184921723729
H	7.08988939902950	7.43810274652675	12.86451226526162
C	5.57605223435474	6.10749733499806	13.73200410139819
H	6.12431719843006	5.21243005248666	13.97864231564039
C	-1.64271545222049	5.61420202001739	10.83289405490294
H	-2.20687202118472	5.50538775859929	11.75851152112819
H	-1.44562076670843	4.62059606901911	10.42849953306148
H	-2.26773623685827	6.13331843821364	10.10552964192744
C	5.10466347715646	9.62732908722986	13.05834778877495
C	0.15423162429461	10.30555293000812	14.89417233240588
H	0.65565104439461	9.35143884509236	15.05963692285889
H	-0.89206100516782	10.18033360619907	15.18029032787242
H	0.61683453623524	11.04077393921495	15.55691291857965
C	0.37453583937535	6.45486110047175	9.69047460596312
H	-0.27284964568779	6.95402913158573	8.96606178610033
H	0.59880141751861	5.45052059068067	9.32228638890705
H	1.30604038840951	7.01114129098726	9.73639699682730
C	3.80356089120743	4.10940297866966	14.97209961116439
H	3.07123327017215	3.47205535612882	15.46816115285625
H	4.61726234882093	4.28563037158237	15.67803924129755
H	4.20153586569518	3.56527730222504	14.11478049656561
C	-0.48450795652933	12.08271983834102	13.28563736786614
H	-0.03366924426487	12.84183888147977	13.92701918689663
H	-1.52649291880688	11.97434047689604	13.58877486343742
H	-0.46588213681733	12.44390935222241	12.25737199840546
C	5.53187312564160	9.88598184474825	14.52473347592822
H	5.62232184676638	10.95799673563637	14.70763043536857
H	6.48747635431456	9.40679324846312	14.75221410889588
H	4.78239960964513	9.49287054681649	15.21123513243664
C	6.21395935721411	10.16442959183433	12.14965657785892
H	5.94113275201323	10.12328348753985	11.09551442731199
H	7.14488163388736	9.61105868892238	12.28695538247496
H	6.42807763839565	11.20721893119286	12.38386416661773
N	6.27816571282339	2.54530962528598	9.94063763706833
C	5.53365291177871	1.40221211524624	10.39954507649935
H	6.07504211109813	0.49285548315084	10.14683669043089
H	4.55819012501934	1.34163865283560	9.91276103845294
H	5.36320939031040	1.40541208857038	11.48283546823814
C	7.68329985624183	2.39092134752666	9.68032148915813
H	7.98150905616019	2.91219173241205	8.76759878716760
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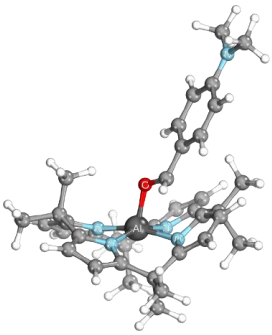
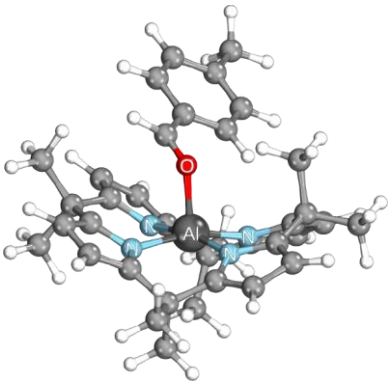
H	8.31951731189085	2.75700476198516	10.49589194408908



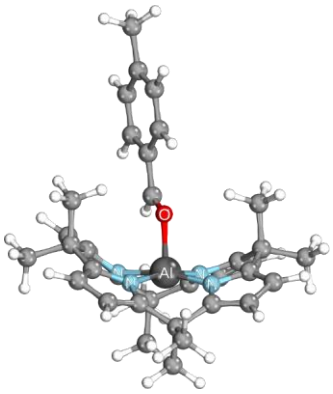
[**1**$^-$]-*p*-dimethylaminobenzaldehyde TS 2 isomer A

C	2.75377985802134	2.16305481080427	1.55382445335326
C	-2.65563629813628	3.26542667474127	1.18534876380471
C	1.49795527708074	-1.92354131721453	-4.42252985924784
H	1.45953426839749	-1.30416771610599	-5.30729814921092
C	-2.07745240845808	-1.51167423864822	-1.06484342821365
C	-1.81610110954439	3.37369935710798	-0.10528602681894
C	1.58121160750867	-3.42626878718510	-2.11051873886119
H	1.61040206556471	-4.02072839659826	-1.20438639431943
H	-2.34486247535955	2.41805246729531	1.79723422695163
C	-2.61665995843398	0.59447809445799	-2.42645708202156
H	-3.04210941536073	0.11760859505422	-3.29676417208388
H	-3.71370174984205	3.13043716743954	0.94855727481723
H	-2.54100355314930	4.16711473957325	1.79040272324231
C	-2.07062833990699	-2.32685337329285	-2.35861055492727
H	-2.94486709127071	-2.07932843532184	-2.96133131185421
C	2.86087398440517	0.61187160943450	3.61539111654041
H	3.78430925451446	0.96832857531061	4.04370776981046
C	2.05059029253381	-0.42580153436192	4.12206048061167
H	2.22985693020382	-1.00774875929141	5.01313243308130
H	-2.12500355944784	-3.39676706039720	-2.14936020953449
H	-1.18760503966750	-2.14483810095586	-2.96465220335983
C	0.08751189550932	-2.57441200360517	4.39302577103488
H	-0.76251666217078	-3.25538835109280	4.46927053813185
H	0.26912997523685	-2.16419596744036	5.38642850932030
H	0.96750195279135	-3.14913859890988	4.10314884965242
C	-3.42586244751081	-1.78471324720188	-0.35285653788721
H	-3.48557885333376	-1.23057309804556	0.58313244133904
C	-2.31221301024320	4.59023801833017	-0.88409055123428
H	-2.22440481011172	5.49602863995849	-0.28297858947506
H	-3.36426608331479	4.47234248324143	-1.14916714765948
H	-1.73931887803136	4.73419580881873	-1.80018522270621
H	-3.55020974240398	-2.84822914903781	-0.13155007558159
H	-4.25291037048380	-1.45957724195091	-0.98639562599767
C	3.74510167720529	3.04501280232218	2.32007784139984
H	4.13797765415620	3.82968495545326	1.67257044755069
H	4.59854307388439	2.45846160950645	2.66275112465956
H	3.27717474169122	3.51354482972356	3.18535161280433
C	3.53305663927465	1.55111808735260	0.37039015960601
H	2.90709244801471	0.92583477177239	-0.25904732680636
H	4.36022121630996	0.93912920809593	0.73832588511180
H	3.94131018005728	2.34693253607685	-0.25680285963313
Al	-0.05125022680469	0.63162992139328	0.67359639279848
O	0.92274706623469	-0.17123118893031	-0.69186378560775
N	1.09160049338065	0.37547621915488	2.25027605041564
N	-1.64035926643140	0.91070670216258	-0.42615035636540
N	0.40941536334011	2.49993812800974	0.66558517456775
N	-0.81642986867471	-1.21413356219651	1.04727186064574
C	-0.36907742398648	3.55251958514079	0.25988939043541
C	-2.03198549399516	-0.03229360939469	-1.35134342145574
C	1.25635376328331	-2.07706731581272	-2.02506055832727
C	-0.51504611434868	-2.02283509074980	2.04748845191367
C	1.61915337011550	3.01942850253658	1.05701989347384
C	-0.20431605277257	-1.45387223992322	3.39827395061606
C	-2.01111480508496	2.13024836032798	-0.92152960308767
C	1.81195256797697	-3.28996207447020	-4.51612144514302
C	0.98343720506317	-0.54013307379839	3.26527922001455
C	1.22754754891239	-1.33530319606458	-3.20336840138958
H	0.97279050177734	-0.28456388758271	-3.15952402210728
C	-1.43083143284037	-0.66897806092015	3.90302694686406
H	-1.68639654274600	0.15557674955576	3.23830469213127
H	-1.21765452762608	-0.24622600937939	4.88579591136913
H	-2.30890909932649	-1.31480751827421	3.98228329151403
C	-2.61064088997888	1.98084305514711	-2.14814488438475
H	-3.00771546968542	2.76537952907402	-2.77343094176714
C	2.24728099153130	1.08197140498310	2.47655223110492
C	1.85598005797185	-4.02930478437485	-3.32065936834268
H	2.10495527823760	-5.08099725463128	-3.32913452030871
C	-1.00016775230504	-1.98360596259187	-0.10260618488349
C	0.33657441896928	4.72427253215683	0.37644885547568
H	-0.01690013750680	5.71615158911776	0.14050746572088
C	-0.84953037443556	-3.34244646885674	0.27771938093909
H	-0.97286334671775	-4.19420843352665	-0.37476617718459
C	1.61017106049938	4.38259927915814	0.88386434989725
H	2.41731602944118	5.06541293953920	1.09859269660670
C	0.97126426413311	-1.44997592804064	-0.72947772399819
H	1.34024449889756	-1.99658492007073	0.14905838854007
C	-0.51842802791844	-3.36963731586702	1.61377497392743
H	-0.28352748535553	-4.23466445427676	2.21399491445456
N	2.06624638444279	-3.88239308056310	-5.72960234628312
C	2.47864701210627	-5.25725162426368	-5.78146271729642
H	3.41686551589041	-5.43982932447700	-5.24496759947087
H	2.63053633212892	-5.55178384228595	-6.81736218226632
H	1.72203187102173	-5.92752118272951	-5.36263773361014
C	2.09239865842601	-3.08202171658868	-6.92326877870867
H	2.29526341079005	-3.71816385946194	-7.78181256066803
H	2.86467987029603	-2.30512608412048	-6.89624454948465
H	1.13316666749358	-2.58900289844730	-7.10440197667415



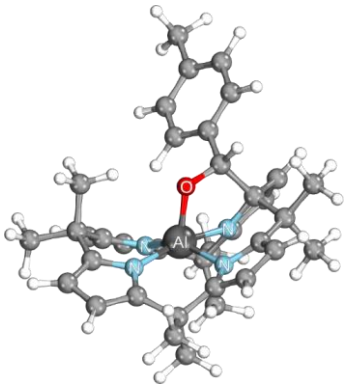
[**1**$^-$]-*p*-methylbenzaldehyde sigma adduct isomer B

C	2.46504449505818	1.80043595090897	1.22553625933433
C	1.49097096774833	-3.11216321394826	3.27000405556012
H	2.06000314892204	-2.70603989860498	4.09701783848653
C	-3.37510378587784	-1.19482784849725	-0.04071576637815
C	-1.73470130038511	3.40719705278459	-0.98656347900840
C	0.02560852375039	-4.10306692118750	1.14598656796384
H	-0.56900512112354	-4.48379533869669	0.32346048358863
C	-3.38372215798335	0.29238480331263	-2.11629508336725
H	-3.99464426727260	-0.33383726350938	-2.74964105920725
C	-3.50179681652874	-2.44856387440596	-0.91192429714964
H	-3.84999714566689	-3.30278726925938	-0.32908540129275
C	2.32814593698437	1.06595715302857	3.68809918500597
H	3.35462108924368	1.24896231948737	3.96397493505572
C	1.31242311670311	0.56817677612411	4.53113398873147
H	1.41161061476140	0.29711023757224	5.57083403575649
H	-2.55697242173227	-2.71905449394169	-1.38321565022127
H	-4.22590782236406	-2.29189077074519	-1.71160555112865
C	-1.10459836176166	-0.68580564272392	5.53659480762192
H	-2.09083457232003	-1.03654689979344	5.84487509387655
H	-0.73822589015874	-0.01034080138802	6.31033505673254
H	-0.43401244915203	-1.54445899296590	5.48889058510402
C	-4.79324906703615	-0.84143849295036	0.47843790444470
H	-4.74712412744235	0.04079633323062	1.11627948083169
C	-1.94371790248676	4.32933815442938	-2.18582305706020
H	-1.59287146034670	5.33771208145838	-1.96328045538258
H	-3.00386147467442	4.39827214789662	-2.43504763824443
H	-1.40585866973215	3.96829219578982	-3.06249486871465
H	-5.21326050374758	-1.66271679821460	1.06385101675414
H	-5.46156684410411	-0.61990570784296	-0.35566985028055
C	3.65993263955950	2.65656207641870	1.66559769309232
H	4.20682929201850	3.02735588277116	0.79819190359838
H	4.36432593102470	2.06687567127701	2.25344696086447
H	3.33963214836891	3.50926737365271	2.26288522413965
C	3.04927361334175	0.63187095214050	0.40308878765666
H	2.27685561631833	-0.01753958609273	0.00360220836392
H	3.71591331489022	0.02559649609878	1.02156782935172
H	3.61910528135126	1.02166813395489	-0.44315003897307
N	0.42324554149430	0.94770399244371	2.49795838920393
N	-2.20961990245541	1.04712882387642	-0.35314090028133
N	0.22173244208718	2.34507941930188	0.17514379757806
N	-1.91669507490640	-0.46266146961852	1.88205711089142
C	-0.27580150235910	3.32154299690586	-0.64993875251406
C	-2.91419339690686	-0.02085141803802	-0.86239570160725
C	0.31862980875086	-2.73518075969858	1.20385506540923
C	-1.73477925223231	-0.89786718205508	3.14944812880910
C	1.54911096583304	2.64092462052253	0.38049154067401
C	-1.18772663895728	0.03085648024445	4.19134176202012
C	-2.28365999725111	2.04642625925448	-1.28543006890398
C	1.19820035614990	-4.46557196752010	3.21982949240949
C	0.16974036673082	0.50889648353175	3.77135135857537
C	1.06004785598338	-2.24445602670773	2.27537812912774
H	1.33689108582191	-1.20233807530732	2.32657832739170
C	-2.14603399576082	1.22917423504286	4.34657652761079
H	-2.23626724517220	1.79772627427948	3.42126720331079
H	-1.77444429863974	1.90818110972912	5.11620718776939
H	-3.14710452163855	0.89400806986076	4.62683657469024
C	-2.98744864049641	1.62114645399110	-2.38435582249018
H	-3.20622705723501	2.19323371825538	-3.27237161056929
C	1.75530236795081	1.29556091916815	2.45707672576629
C	0.45930633086384	-4.95368362785463	2.13349240045414
H	0.22261484086974	-6.00991009550239	2.07899785690675
C	-2.54776742327032	-1.47067113906751	1.18928225957074
C	0.71562967882828	4.21094659853658	-0.97848930076258
H	0.61694440217580	5.08387313688487	-1.60476113607892
C	-2.72973248323967	-2.55541240003353	2.04158961222847
H	-3.21956797570181	-3.48608575395262	1.79575871899431
C	1.88489936407605	3.77327627601712	-0.32124457749713
H	2.85412829670597	4.24505608651829	-0.35957341190065
C	-0.16461181570261	-1.88280945983562	0.14126368120040
H	-0.64914163443157	-2.39455203617155	-0.69903823793913
C	-2.21357019469005	-2.19523326556653	3.28796051023973
H	-2.17809091024633	-2.80333169137739	4.17778392122893
Al	-0.73433860148148	0.82429702964823	0.90799874160119
O	0.07965416272003	-0.67033771375298	0.02301723612282
C	-2.50189363373784	4.01119318853141	0.20895894653641
H	-2.12633472656717	5.01128235627352	0.43480293116661
H	-2.38828236536018	3.40740755162887	1.10996762006821
H	-3.57019831986230	4.07572195848768	-0.01026350621145
C	1.64069904060108	-5.39742954579461	4.30789503369424
H	2.14172571122985	-6.27806912550412	3.90253559341922
H	0.78710250076273	-5.75214149234782	4.88933404740694
H	2.32794392051935	-4.91025677079672	4.99815988917219



[**1**$^-$]-*p*-methylbenzaldehyde sigma adduct isomer A

N	-0.49157569367296	-1.78690090090893	0.42600660118206
C	-1.47205439998767	-2.51838085827530	1.04879003979750
C	-0.51928696102648	-2.11820890153511	-0.89852335236606
C	-2.15122795649269	-3.26574123729247	0.10496846019634
H	-2.95544944008435	-3.96083991407014	0.29758367406886
C	-1.53330049902037	-3.01966482064094	-1.14114286256673
H	-1.78220504704774	-3.47293764501446	-2.08837827603130
N	0.13100955027453	-0.81042673719925	2.84899902093994
C	0.96101632229821	-0.41000567588670	3.86253282973099
C	-0.60023791914071	-1.87214456868507	3.32379529567522
C	0.74762084121952	-1.18548558577995	4.97565714441072
C	-0.25380541557128	-2.11738630066238	4.63218725371793
H	-0.66774583672004	-2.87782169811078	5.27683692921468
N	0.77478563209303	1.64750931765908	1.73739787208236
C	0.63678683848850	2.89660463016889	1.17968511043469
C	1.51807532470479	1.79740833615296	2.87956383474517
C	1.25586314713458	3.82543307429782	1.98213043326988
H	1.31417466201566	4.88908562518264	1.81138020192718
C	1.82335146538121	3.12231673247889	3.06672086542718
H	2.40770336954409	3.54287722431630	3.87020581115910
C	0.26646828025891	-0.02737851790365	-1.87330668758376
C	0.02809372220399	2.01747744953156	-1.07765684108978
H	-0.69833515741155	-1.87982263509924	-3.64171953282690
C	0.29160295928003	-2.10085605340028	-3.24139046994044
C	1.90655458968845	-1.84175612714503	-1.37809797557808
C	0.47520357505115	-1.51448546084306	-1.84421566237755
H	2.06637609010807	-2.92168235953297	-1.34362140618316
H	0.42008920889476	-3.18431567506393	-3.22078687205678
H	2.11325735141981	-1.45115422976938	-0.38166465773951
H	-3.14911322260975	-1.03390512443002	2.89938011913475
C	-3.05756398789161	-2.11476949650277	2.97665736183828
C	-1.57809346652956	-4.10342330025980	2.91376739244526
C	-1.66068368698588	-2.60775341041879	2.54662161187909
H	-0.61218032252088	-4.51649898002118	2.62677015990358
H	-3.84566931605498	-2.57205230516957	2.37346405758167
H	-2.35686776863122	-4.67254076778433	2.40406663755943
H	3.98620574423967	0.68384129655113	2.65781688042627
C	3.18391005582757	-0.03655379244579	2.83098350928430
C	2.61417015410969	1.06260433833474	4.97863833632467
C	2.03697872556451	0.61125866083301	3.63804399185781
H	3.02999976645928	0.21495860824456	5.52477672820731
H	2.84605438965854	-0.38727989284350	1.85438962840365
H	1.85095160404202	1.53067596945943	5.60031000565074
C	-0.10499797864656	3.16620571052491	-0.10382117218273
C	-1.58377236010199	3.50578585013730	0.18782767438002
C	0.49538728908641	4.41888392824594	-0.76067050425078
H	-2.13994876981084	3.63756842935848	-0.74323673190412
H	-0.04620133770290	4.67773686427966	-1.67140062522983
H	-2.07695198648603	2.73738130897804	0.77451021043227
H	1.54363506801167	4.26736939018552	-1.01343758874496
H	-1.64413789683486	4.43255730034092	0.76279459795354
H	0.42104627472809	5.27876771633876	-0.09446465751808
H	2.63500422030973	-1.39954125678605	-2.06027437081526
H	1.03139741178095	-1.69095087565951	-3.93010339456221
H	-1.71095132301183	-4.25580448295234	3.98559728366861
H	-3.23420580850286	-2.37176610671970	4.02276318480241
H	3.42235942637253	1.77939348036883	4.82812390230373
H	3.58914139659464	-0.89902619745839	3.36455224021076
H	1.26067202423677	-1.11180991065331	5.92177571196211
Al	-0.04750990180642	0.01880696226608	1.11084152262136
C	-2.73414353515775	-0.01348393793365	0.03878082553888
O	-1.96854613437610	0.45803875392987	1.17874634623776
C	0.04851466521651	2.11564228498666	-2.45104282684032
H	-0.02210247606175	3.02131870104217	-3.03292026980353
C	0.20442808342034	0.80898841735286	-2.96025479101795
H	0.27680067372118	0.52505218074997	-3.99884318399763
N	0.14872658900082	0.69535490642097	-0.71565867816870
H	-2.35498991947054	-0.57798904692266	-0.52253096454727
C	-4.17021850950738	0.19861071617942	0.40162607035954
C	-6.94013551742742	0.54085885730156	0.45167239864073
C	-4.75515302317606	1.01878806313101	1.36637512645249
C	-4.97391815166805	-0.44732329309841	-0.53319696178331
C	-6.34622488443314	-0.27682082276752	-0.50578322114450
C	-6.12469962612149	1.18678422036657	1.38274875597098
H	-4.13083090454634	1.52136187099090	2.09340983837086
H	-4.51232363583694	-1.09350514097693	-1.27035613516338
H	-6.96529117531678	-0.78429119357550	-1.23537713853427
H	-6.57490375504033	1.82952714542539	2.12953656691231
C	-8.42972637907619	0.70309805923579	0.50490190597597
H	-8.71308417225276	1.70394925584707	0.82981992078212
H	-8.87025995066936	-0.00360588166330	1.21145492627607
H	-8.88986628199779	0.52224748266637	-0.46587399578027



[**1**$^-$]-*p*-methylbenzaldehyde 1,2 adduct isomer B

Al	2.05107714057677	8.03603821908846	12.55709166155091
O	3.09318121886783	7.95256535160274	11.09965959816986
N	3.73629402351848	7.43147264412106	13.48073250934443
N	0.25621940997166	8.51893081892826	12.12525764889069
N	2.54528998393558	9.82940077533252	13.15023357404573
N	1.41830412270449	6.21799579168066	12.99685082566957
C	1.71788567081662	10.90921900815570	13.02027441750385
C	-0.64268303280081	7.68695727140234	11.50997130916207
C	4.90851206861915	6.42720303962190	10.74610791255481
C	1.93325526330359	5.29369835676658	13.86771569749764
C	3.83150265118347	10.28401637881957	12.96722659817300
C	2.99340876012349	5.63733107716140	14.88968374010753
C	-0.37232185527876	9.71339914749430	12.34992398169423
C	5.87022706819284	3.90497990019742	9.93128563697427
C	4.06393222646010	6.40840093601065	14.17390260455584
C	4.12651654728525	5.28764759126036	10.89393859646292
H	3.13474989741386	5.35514167327810	11.32005986907690
C	2.41292804638430	6.52824023807885	16.00379859953473
H	1.97826848527794	7.44327284234330	15.60337709210856
H	3.17894035132406	6.81124837779816	16.73088004340527
H	1.62406749167065	5.98613752052300	16.52579230416743
C	-1.65313021274772	9.65614714225666	11.85349032880489
H	-2.39650958595932	10.43746418815545	11.89347849227297
C	4.86705206150455	7.96227887161863	12.77378237429945
C	6.64054065661158	5.05141886679057	9.76367291023914
H	7.62249471260520	4.97683888565465	9.30865903771523
C	0.45638705508501	5.58390653235204	12.25699952304834
C	2.45678768957641	12.04073248331766	12.76582191571437
H	2.07967750355647	13.04047039801253	12.61805795040320
C	0.36744520058502	4.26518223687848	12.65126529802109
H	-0.29813031672735	3.51580033803429	12.25278798240364
C	3.80964255555711	11.63834120880910	12.72534174591408
H	4.66122768540367	12.28057881872091	12.55782696553905
C	4.43880366029333	7.78344974365779	11.23941262148842
H	4.99599555157162	8.54461863055376	10.67118683703745
C	1.31267267932194	4.07962041958632	13.68270334697576
H	1.49898121965119	3.16609625230364	14.22666442705364
C	4.60936447903618	4.04860323667631	10.50080607381937
H	3.98092581887293	3.17650055208016	10.64190492774604
C	-0.30130543193422	6.26614913235760	11.13809932987630
C	0.23465226241052	10.78056979067698	13.22448643918018
C	6.16339265625139	6.28986180602176	10.16279487287516
H	6.78140340124272	7.17053558360720	10.01708029991749
C	-1.82529092164415	8.36051721582963	11.31449129111937
H	-2.71963265314424	7.97432996030412	10.85068887937901
C	5.98219816131700	7.07322904659791	13.21762869037588
H	7.00885252776494	7.16285412873757	12.89600643886894
C	5.49734426827569	6.15488905792272	14.06394538385703
H	6.03597221646662	5.35006646547003	14.53916596316491
C	-1.59725483602378	5.49392662325053	10.87555520477366
H	-2.23265764492400	5.46537186258390	11.76036822233581
H	-1.38139451234959	4.46894274096228	10.57097798629986
H	-2.15808309799755	5.95682783116908	10.06274875097001
C	5.07016008593243	9.45188882857992	13.20366736016015
C	-0.02887909994321	10.40897330623952	14.70013656280481
H	0.41399296493133	9.44457917416626	14.95026431048428
H	-1.10170434862734	10.33689267152323	14.88931654958447
H	0.39980025321026	11.15744704693662	15.37108441533361
C	0.51852364947188	6.22776168062140	9.83098910505540
H	-0.06027633562348	6.67392478553911	9.01920604479014
H	0.75496617422627	5.19525033200946	9.56133060043278
H	1.45438690510396	6.77574939876526	9.90794017192270
C	3.57039571002897	4.37304232001660	15.52005812050506
H	2.78986754272583	3.82375211764479	16.04544484730464
H	4.34468497388542	4.61764234017592	16.25029607113555
H	3.99840391706720	3.70884122169073	14.76867902472092
C	-0.44306574934320	12.12198595661740	12.94970849962689
H	-0.03742978613154	12.89992973344751	13.59874481273131
H	-1.51390559543270	12.05992906502297	13.14538751764114
H	-0.30505924086777	12.42931959632596	11.91319629935673
C	5.39623393208539	9.50934678520059	14.70882560630263
H	5.48846450084643	10.55344781378818	15.00759184061423
H	6.33141727831381	9.00078022762603	14.95567644062089
H	4.59809145063470	9.07457197348333	15.30943883088892
C	6.36798551422973	2.56421338567844	9.47213817258143
H	6.16759537185926	2.40719471326764	8.40969679854556
H	5.88393632475360	1.75162524341227	10.01404966517240
H	7.44459015211525	2.46194954307552	9.61505461230264
C	6.26191385199209	10.04860570664970	12.44927682653451
H	6.07071289223508	10.14582769108118	11.38187266622159
H	7.16511663449456	9.45048080945055	12.58703698512748
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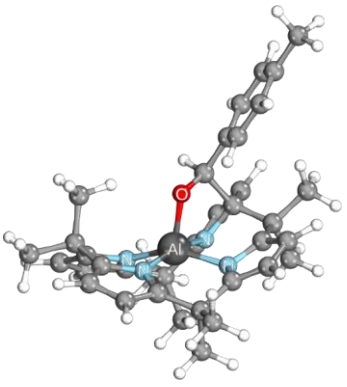
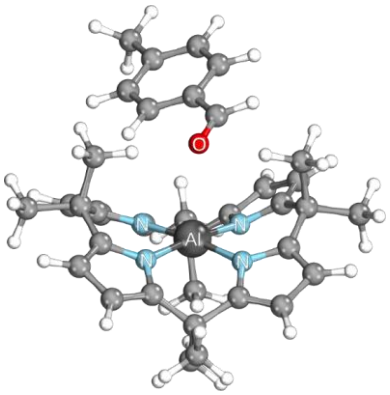


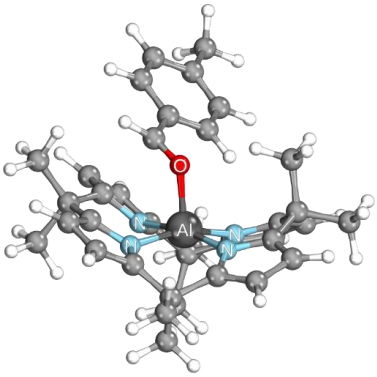
[**1**$^-$]-*p*-methylbenzaldehyde 1,2 adduct isomer A

N	-0.05427955098993	-2.32109936282062	0.41245545096832
C	-0.25879245645221	-3.50647676357867	1.06526326116478
C	0.37942877013645	-2.62922938681786	-0.85110527108938
C	0.04651715312572	-4.55625043216106	0.22631040643956
H	-0.02048205096487	-5.60773593369748	0.45664598614196
C	0.45558390553266	-3.99445714000823	-1.00141711702022
H	0.77136868739301	-4.53370634880970	-1.88169912673171
N	0.04357392272648	-1.25763924099242	2.93176705556574
C	0.65576705253985	-0.59142131333197	3.95869642101120
C	-0.19236941289181	-2.54079580144450	3.35387426052938
C	0.78372696012673	-1.43265044627001	5.03795478584853
C	0.23908735253026	-2.67923423171192	4.65160522124959
H	0.18767854151341	-3.57050760536608	5.25790312483171
N	0.04273559677763	1.27194004982111	1.64421157514930
C	-0.67654003196765	2.31436353232643	1.10028180454855
C	0.40187262395346	1.65565816998532	2.90654821467584
C	-0.77037250536233	3.33718114253375	2.01403115040884
H	-1.26420378978638	4.28633059505275	1.87136025648177
C	-0.07544954587888	2.91804779018457	3.17081953839073
H	0.05518194528173	3.48139714818681	4.08151301560095
C	-0.27731267097244	-0.50291102666131	-1.81927521745567
C	-1.63732776162322	0.98510091801584	-0.83684589716562
H	-0.07406604014160	-2.64633216137227	-3.56863908296036
C	0.86323831080546	-2.17920757660762	-3.26547723162064
C	2.12608468203849	-0.94610782387915	-1.50552273326004
C	0.76754570386990	-1.57822081426757	-1.86575795182670
H	2.89744949940032	-1.71635030257279	-1.52359682965499
H	1.63921161462787	-2.94312008545207	-3.29583744722555
H	2.11457466991715	-0.51111499497649	-0.50667526753924
H	-2.65442180233954	-2.42357980536852	2.02936675317748
C	-2.36151545941295	-3.39517458288366	2.41993271096806
C	-0.55970128856464	-4.96772682642805	3.04368329341093
C	-0.82944572345980	-3.57722274666091	2.46333170460036
H	0.50804865931446	-5.17903372574461	3.09795070981498
H	-2.81418768874052	-4.16312016233488	1.78779768734313
H	-1.03501331111795	-5.73832140483111	2.43517454416364
H	3.11135350479720	1.58471673553658	2.93455593631091
C	2.63863998175370	0.61192517326134	3.09080566654578
C	1.48253560212000	1.43758528140963	5.12722666079731
C	1.26113705369895	0.77495352730797	3.76865856792869
H	2.15020459997508	0.83639622359233	5.74490425552001
H	2.54702917198233	0.12588057182453	2.11934993968998
H	0.54277803396525	1.56065851717708	5.66528539724901
C	-1.09483736246618	2.37111335069564	-0.34729940705753
C	-2.10524143457505	3.49834357327860	-0.58443666561860
C	0.15880553537320	2.73541030921192	-1.17360341292772
H	-2.42958061728152	3.52649225171958	-1.62617184997261
H	-0.05368449858804	2.81827891937877	-2.24270287357448
H	-2.98777534112609	3.43075812242992	0.04345978558674
H	0.96692357567766	2.02023440006375	-1.03233369378926
H	-1.62774726611599	4.45696914656169	-0.37822342717166
H	0.52665126191993	3.70175520431828	-0.82830074391685
H	2.40418266045592	-0.15856939262686	-2.21135531893718
H	1.12867475478589	-1.41744669767891	-4.00169088148117
H	-0.97822517729752	-5.04941385328138	4.04742500569159
H	-2.77425581685134	-3.48654587734074	3.42721215369820
H	1.94362796447068	2.41933790330077	5.00654836466252
H	3.29506865178764	-0.00511095925176	3.70739385154911
H	1.23816749062999	-1.19883470446074	5.98844246806112
Al	-0.47448534494730	-0.57337320172766	1.22794156946453
C	-2.77711300490675	0.24771863701845	0.02717732399369
O	-2.24475705659541	-0.28362967387168	1.16263678895934
C	-1.93345226716095	0.94075398305479	-2.29684769152748
H	-2.68960546333356	1.53558990762049	-2.78774144249704
C	-1.11878522038744	0.04764267146058	-2.87890185851653
H	-1.09209308102503	-0.23979649709690	-3.91897284035626
N	-0.56141802108575	0.04202142021585	-0.69869884544410
H	-3.12826829171594	-0.54533550429843	-0.65955641630296
C	-3.96441206169042	1.13239278796265	0.31935875199020
C	-6.14480129497741	2.83484449303083	0.84102342698743
C	-4.12541900182100	1.71083218426845	1.57336432484650
C	-4.92049292462987	1.38879114711058	-0.65507891239756
C	-5.99072927340533	2.23367224082142	-0.40360962208335
C	-5.19749494645410	2.55319938599610	1.82162382335521
H	-3.39112739855066	1.51504568971967	2.34243549825611
H	-4.83067923179993	0.92000568985788	-1.62963362552310
H	-6.71935186016960	2.42291008803670	-1.18440048421142
H	-5.29581159037188	3.00606868065112	2.80201203677027
C	-7.31814852011079	3.72636175403734	1.13172085384417
H	-7.06329048335141	4.50003321467747	1.85646802675219
H	-8.15541316671646	3.15987400006123	1.54665733076426
H	-7.67932738482898	4.22346393137000	0.23089344509674



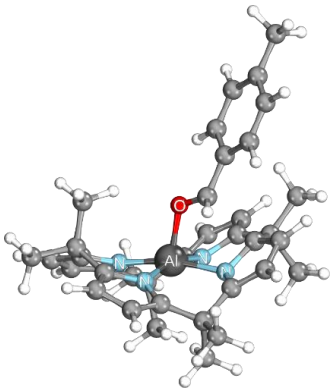
[**1**$^-$]-*p*-methylbenzaldehyde TS 1 isomer B/A

C	2.49075698050897	2.36553454895637	0.85601602268032
C	-2.75127396231476	2.76969398364812	2.50567853009003
C	1.15969964966322	-4.08985697209802	-1.98687847457631
H	0.24719051753227	-4.67212887539690	-2.03362758543008
C	-2.65376582730477	-0.27065695502273	-1.98296548516708
C	-2.36214064897048	3.54491873013078	1.22678112361177
C	3.46597060302658	-2.57953033667538	-1.81621144061504
H	4.36778086804327	-1.98477974560907	-1.72580477926167
H	-2.28325648116374	1.78379522724883	2.54508077337064
C	-4.07673521589840	1.83917255987060	-1.56833550382773
H	-4.86699774865662	1.65542816363225	-2.27906659517239
H	-3.83133439529884	2.61548306162201	2.54829769674418
H	-2.43276492986329	3.31486576360107	3.39645546409304
C	-1.68800386280712	-0.02668223222267	-3.16035604345014
H	-2.17797190604746	0.59283468258662	-3.91455745842283
C	3.26536486983511	-0.04419216259001	1.33831553151422
H	4.33030117007132	0.13345843984948	1.35232424684639
C	2.61724972945163	-1.27422871124993	1.60790335770459
H	3.09158174444438	-2.21197485240860	1.85125764629791
H	-1.39528114759598	-0.97165631120216	-3.62481639944443
H	-0.78327140708492	0.48718991794589	-2.85271946733740
C	0.64031170128938	-3.34718149855378	2.14324034503051
H	-0.18013215953620	-4.01489056355826	2.40902544598466
H	1.33500400398891	-3.33123898079942	2.98442123180879
H	1.15451582732410	-3.76525241977060	1.27712631288962
C	-3.92505294235301	-0.88531804864356	-2.57698197656967
H	-4.66926069818494	-1.08577137813053	-1.80707275691976
C	-3.06490019734892	4.90029898553812	1.27705392383482
H	-2.76432938728939	5.45827778161945	2.16452282990833
H	-4.14682271861018	4.77226904453133	1.32738171397850
H	-2.82932574419172	5.49977957438171	0.39799224758106
H	-3.69647681158003	-1.82040714239957	-3.09050958336634
H	-4.36556539809092	-0.21636969374749	-3.31677564077696
C	3.62767798242446	2.85535865609914	1.76579044821037
H	3.83527927694558	3.91300880513372	1.59778652727619
H	4.55091032499414	2.31318681091273	1.55888092192080
H	3.37732726543305	2.71451612978040	2.81625105366153
C	2.47371461540609	-6.22780555485499	-2.07687654866456
H	3.49416427313578	-6.57328772515164	-2.24027296793419
H	1.85531542871314	-6.61891453213248	-2.88583401490903
H	2.11633996981132	-6.68329388856062	-1.15127672374750
C	2.93087231045844	2.63622740403965	-0.59801226025560
H	2.15271333551206	2.37605654162426	-1.31153526242435
H	3.83357263344509	2.07015150458671	-0.84451606153521
H	3.15166663349091	3.69786614838683	-0.72390451341731
Al	-0.53371229586376	0.93702816884442	0.34134599946069
O	1.15570064754959	0.16215787298351	-1.63043718754813
N	1.05334833037490	0.28440091668019	1.21157088001589
N	-2.20077007214160	1.60678437264121	-0.35476303575869
N	-0.01965342535349	2.71130916809539	0.88936171520429
N	-1.17349669568801	-0.85420111773995	-0.00359451964191
C	-0.87661459166856	3.73845337992246	1.20437534857112
C	-2.99506465240538	1.03340845546540	-1.32152653825771
C	2.22627071561376	-1.95036617647705	-1.79986401454732
C	-0.83974906740674	-1.98452628664057	0.69691223605592
C	1.25362638283451	3.16417865420581	1.14745028772698
C	0.12020713664308	-1.94107129388833	1.85108889205601
C	-2.82418114415320	2.77062134037469	0.03011044156901
C	2.39727141076092	-4.73117404979141	-2.00166461144111
C	1.27053125438861	-1.03120832368675	1.53149138423006
C	1.06613434987111	-2.71519693852475	-1.88902171904268
H	0.09404298419120	-2.24070135340886	-1.87256528487358
C	-0.60287136925491	-1.42988655842985	3.11397895428185
H	-1.00928525913035	-0.42656835623122	2.97700617162970
H	0.08445184449988	-1.38713837935077	3.96136585887195
H	-1.43688040128101	-2.08731971881359	3.36714403476890
C	-3.97047504441615	2.94853625378234	-0.69918261303505
H	-4.67322834141407	3.76150292808020	-0.60562246446896
C	2.28222886795027	0.89413310022902	1.12523158491741
C	3.55180045722570	-3.95651023424334	-1.91895272693945
H	4.52235793744959	-4.43827519892359	-1.92401945946650
C	-2.07709871106576	-1.22760789360507	-0.97112298170001
C	-0.16280951803901	4.82626423368329	1.63587981415168
H	-0.56541427392995	5.77147045638086	1.96457022135043
C	-2.31542715446119	-2.57986496269866	-0.87197225248986
H	-2.98236816361423	-3.16098314677826	-1.48942737812185
C	1.20011106637760	4.46041687699633	1.59484239741696
H	2.03834534765478	5.08552680783793	1.85992344050142
C	2.17356514200954	-0.49158638761388	-1.66737896989665
H	3.15681625801324	0.00556972619954	-1.61363656666705
C	-1.53146473765913	-3.06165707607672	0.19999011185554
H	-1.47686233921932	-4.07987009942765	0.55243769744803



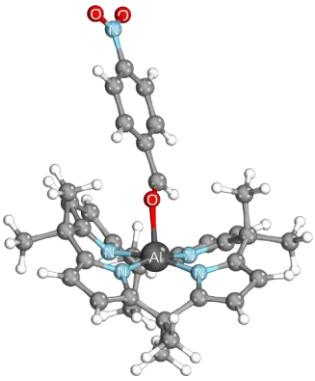
[**1**$^-$]-*p*-methylbenzaldehyde TS 2 isomer B

C	2.45417427527804	1.81886437940398	1.26738956656421
C	1.49842080339555	-3.15397772396313	3.23948979075134
H	2.07817334932513	-2.75221482931321	4.06159882476064
C	-3.33155478084609	-1.21174078899151	-0.03249612987921
C	-1.71742449217581	3.40094942651808	-1.00956505911285
C	0.00870437404701	-4.12753447255732	1.12944312838299
H	-0.59236275245308	-4.50692274002845	0.31036053752780
C	-3.36607671662361	0.27390009666614	-2.11300284401889
H	-3.96667100620788	-0.36112772717411	-2.74726696082025
C	-3.51609658032958	-2.44955967514919	-0.91475696668687
H	-3.83163954476992	-3.31316424175081	-0.32672749741546
C	2.26935454911703	1.13139380445372	3.74407613504542
H	3.28777746517177	1.32638402245915	4.04068115724656
C	1.24003034472063	0.63197293555026	4.56967804294963
H	1.31928887454783	0.37418626830283	5.61449575004067
H	-2.60616866600829	-2.71468581077547	-1.45284536578942
H	-4.29016332681439	-2.27501556881921	-1.66194115445642
C	-1.19000869068490	-0.62736489588080	5.54280157925660
H	-2.17891256277521	-0.98518730502829	5.83472880638402
H	-0.85032126878329	0.06458771103635	6.31376982944952
H	-0.50710888651463	-1.47730959047395	5.52482190130102
C	-4.71564220621233	-0.85279491524180	0.56600446228271
H	-4.62845557446057	0.01416322350880	1.22030879505939
C	-1.91962587574969	4.30782595536303	-2.22171068166125
H	-1.56450233081840	5.31735424961914	-2.01174587758394
H	-2.97875746863107	4.37863601895165	-2.47481500896941
H	-1.38096684403568	3.93260650320736	-3.09188971913682
H	-5.12218818752508	-1.68195504673075	1.15030954986247
H	-5.41862839462201	-0.60217297760835	-0.23027790340594
C	3.64869637518512	2.67323917265369	1.70956652008285
H	4.20950577755023	3.02534885978710	0.84318173160339
H	4.34043994361542	2.08813477410987	2.31672858515835
H	3.32721297270123	3.53849214619200	2.28812363849263
C	3.03729770836367	0.62978758985311	0.47413543842227
H	2.26477945098273	-0.02754161940073	0.08703583395485
H	3.69847693159791	0.03603010931449	1.11031108045782
H	3.61349748265015	0.99854526345489	-0.37729239562234
N	0.39487789810318	0.97669186309767	2.51234338394490
N	-2.20262745749104	1.04775375443702	-0.35079785601305
N	0.23478932779571	2.34873777782533	0.16857530466384
N	-1.89109189848551	-0.47359790453729	1.87797871811337
C	-0.25838154118320	3.31802040157165	-0.66640606820596
C	-2.89595520715131	-0.02936377940836	-0.85699457059173
C	0.25152558178061	-2.75236807186141	1.21984876453267
C	-1.76335228795323	-0.87751123886447	3.14286931000847
C	1.55554802607846	2.65254630666450	0.39601207461583
C	-1.24834927039861	0.06894168165486	4.18572076022435
C	-2.27464399986506	2.03886032557480	-1.29156316946073
C	1.25650099696806	-4.51498281290858	3.15676569817914
C	0.11569762039449	0.55099744573189	3.78463726533875
C	1.00989417735200	-2.27226648727845	2.28177998182476
H	1.25072805083863	-1.22277383952363	2.36041395251510
C	-2.22296659402567	1.25891045364612	4.29548882109144
H	-2.29418721130589	1.81032656559338	3.35835110835398
H	-1.87518320648825	1.95328701562264	5.06201101509739
H	-3.22806981973748	0.92093982878645	4.55831893219330
C	-2.97478602179878	1.60265052077973	-2.38897523527949
H	-3.19132747458430	2.16602401612272	-3.28305167428976
C	1.72287660215122	1.33715890351871	2.49691829996137
C	0.50475424829806	-4.99295373704680	2.07513456882177
H	0.30975469452215	-6.05583384210962	1.98749113130698
C	-2.43651122633277	-1.51595591830163	1.14936294480069
C	0.73331832808792	4.21242499738879	-0.98236932931035
H	0.63928094259261	5.08364379553586	-1.61186937470289
C	-2.65737741608501	-2.58931653148224	2.03159201414938
H	-3.09813666398640	-3.54141028933617	1.77549530111791
C	1.89543770800305	3.78450599697815	-0.30477862416532
H	2.86196705363440	4.26284809637166	-0.32892341585693
C	-0.30001072890371	-1.87165285297056	0.20078223950108
H	-0.77615239302489	-2.37135181309179	-0.64934818136099
C	-2.22409608896510	-2.19793193709095	3.28390898280778
H	-2.20426614281823	-2.79149765433254	4.18373746160532
Al	-0.70926475451859	0.82470163706209	0.88831015500119
O	0.06057191094473	-0.67268983518601	0.05298808886865
C	-2.48390699999653	4.02409611777589	0.17660035483970
H	-2.10477894127235	5.02566334947529	0.38940247566143
H	-2.37225843953642	3.43173590597284	1.08535338160336
H	-3.55182430517536	4.08970929886199	-0.04455750123909
C	1.77408446206766	-5.46589387582059	4.19517013005121
H	2.36337831695348	-6.26763889329780	3.74627701163230
H	0.95545630254457	-5.93746794982009	4.74287725087202
H	2.40580932076473	-4.95796937329961	4.92277099669872



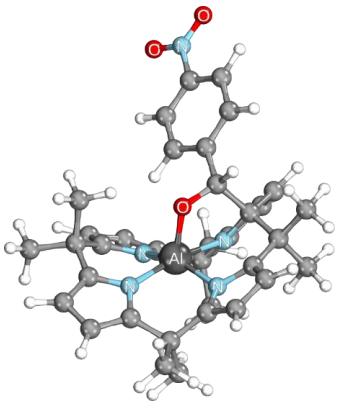
[**1**$^-$]-*p*-methylbenzaldehyde TS 2 isomer A

N	-0.69667751703837	-1.53484396052680	0.13436557343148
C	-1.89805823304338	-2.01875218198553	0.64700792488105
C	-0.60172379603690	-1.91867619186096	-1.13061084303403
C	-2.52180637798250	-2.77150319975878	-0.37587662961839
H	-3.45209172178986	-3.31166265702102	-0.28053273499021
C	-1.72433853078589	-2.69073969272250	-1.49912345879893
H	-1.91952128820383	-3.11084557445389	-2.47325578200498
N	-0.15758461724900	-0.65557334488821	2.64332733081696
C	0.37191365701158	-0.12645071082189	3.78821882258150
C	-1.23661868668549	-1.42539149813195	3.02098924666977
C	-0.36063792633767	-0.52772242744643	4.87810354983519
C	-1.39690792427722	-1.35323898452646	4.38449647080497
H	-2.14081445736115	-1.86807415935906	4.97384432261975
N	0.82645909217386	1.77076303658572	1.61916856786958
C	0.96095949888303	2.98401260636771	0.98857346388107
C	1.45941787615394	1.87440492483298	2.83068212674893
C	1.65592710513353	3.84768322776581	1.80037752227060
H	1.91384821514411	4.87206766006462	1.58155228407456
C	1.97767722868660	3.13665534395179	2.97803439227201
H	2.53560552686967	3.50997499318528	3.82283244610721
C	0.59173979705115	0.01023465668451	-2.01048786097598
C	0.55092512397632	2.09289686998102	-1.29357409945410
H	-0.39276782059988	-1.72392342833873	-3.88935305947646
C	0.48727163520606	-2.08446536956846	-3.35618782850611
C	1.86529162692268	-2.01725366371071	-1.29024700424960
C	0.57616891451670	-1.49251059939165	-1.95191034371322
H	1.85809019208043	-3.10781016498335	-1.22050715482649
H	0.44501162917904	-3.17456200866495	-3.31387507640851
H	1.99533901493872	-1.62355830719974	-0.28259457718608
H	-3.96272070090610	-1.84010832821861	2.62565012330665
C	-3.33428317507464	-2.72554851113896	2.58868379370514
C	-1.09811852902298	-3.73061052730302	2.19512829575289
C	-1.91499943049327	-2.41698474520202	2.11035926973891
H	-0.07423348842731	-3.56736408542364	1.86084889177495
H	-3.81733307601276	-3.45918845947043	1.94074604240129
H	-1.54163957723641	-4.51431963938665	1.57510239082702
H	3.71367971431692	0.37691437477893	3.18377384599513
C	2.78281121342713	-0.19296285992199	3.21408811261143
C	2.00295299452342	1.15702057364401	5.14339439166146
C	1.62989008641371	0.68906783413027	3.73830975653202
H	2.13388832628361	0.30277381318615	5.80975428963700
H	2.58706901260976	-0.55470926271280	2.20414489507816
H	1.23401325132645	1.80647534387489	5.56184175908744
C	0.37500223642692	3.27159134004958	-0.36821258494111
C	-1.11506194534085	3.65596969522135	-0.24798354677959
C	1.09049447806934	4.48521499681799	-0.97162321874995
H	-1.53062304761456	3.87211011228867	-1.23517272601186
H	0.66330392905975	4.74240687435019	-1.94169112119543
H	-1.71133700947507	2.86842864978964	0.20247935871207
H	2.15571393274713	4.29683609544251	-1.10128549115395
H	-1.22031321698305	4.54601885292607	0.37643236826293
H	0.96965839075048	5.35862949916236	-0.33000006720700
H	2.73138089288863	-1.71005486539895	-1.87805178850818
H	1.36625501006705	-1.81231534043440	-3.94050978582762
H	-1.06062869659554	-4.07947739004744	3.22852757377123
H	-3.30921057678216	-3.15737077364657	3.58936872127894
H	2.94303948612285	1.70974899786726	5.12911685928033
H	2.92361752281066	-1.06642103494122	3.85508667278240
H	-0.17705147620418	-0.27157396522122	5.90992746358985
Al	-0.12169138525476	0.25154838095915	0.91807754674762
C	-2.74825270627874	-0.02953339286015	0.30236104792462
O	-1.94176216486911	0.69649746790083	0.96557542837783
C	0.83233942640965	2.13600481745954	-2.63999326836576
H	1.00326904794283	3.01936807854871	-3.23460337432002
C	0.85976736396041	0.80256220373728	-3.09920456509521
H	1.06292692871164	0.47120993926457	-4.10597036987225
N	0.39566638434073	0.78659292843279	-0.89689445413397
H	-2.55852510861492	-0.22434732135369	-0.76141152109043
C	-4.16328869890385	-0.03022494645210	0.70727296624521
C	-6.86695437124055	-0.00475151771615	1.45112390791099
C	-4.55761186323527	0.55338903045225	1.90991573925674
C	-5.13052410533787	-0.58704987008465	-0.12169010930072
C	-6.46456992048701	-0.57363678015295	0.24565619454463
C	-5.89249084531391	0.56029511314603	2.27145233370948
H	-3.80820363623734	0.98396358180112	2.56083462396986
H	-4.82813387749243	-1.04171573010367	-1.05786647210010
H	-7.20590456918690	-1.01140717747306	-0.41264524927709
H	-6.18439177703367	1.01271886047123	3.21226850060800
C	-8.30769092436853	-0.01384985678843	1.87100704459638
H	-8.61682671679863	0.95627559521549	2.26189764215141
H	-8.48385444634568	-0.74893759136928	2.65919932330365
H	-8.96766580257727	-0.26225427215523	1.04021494717503



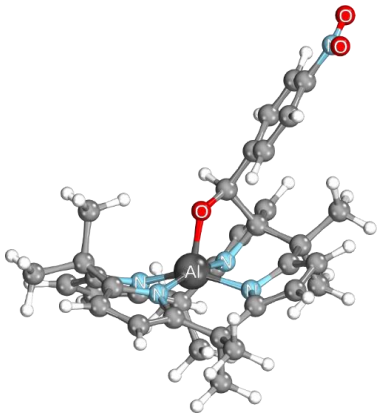
[**1**$^-$]-*p*-nitrobenzaldehyde sigma adduct A

C	2.60825345550881	2.10468828782932	0.88175673065372
C	-2.49973982632870	3.32395835938359	2.21387875902023
C	1.62258510209993	-2.94109616738748	-4.00370636776098
H	1.21140673384503	-2.94484157148258	-5.00206876105362
C	-2.78619748136487	-0.75806352499564	-1.43949171089778
C	-2.12593636920451	3.69293611478179	0.76004736042816
C	2.69217029261754	-2.95724198721818	-1.43817607496351
H	3.09264691884522	-2.95645175116161	-0.43173097713520
H	-2.09420497486668	2.35269734126955	2.50342908042528
C	-4.10414285927819	1.43315754424834	-1.38637370627699
H	-4.94476590865956	1.12190164785754	-1.98761756293370
H	-3.58432325403915	3.27190078332695	2.32941625134345
H	-2.10148095030141	4.06291865821285	2.91215592653739
C	-2.25912044364894	-0.76978565153521	-2.88675914998996
H	-3.00950793667969	-0.35237371471377	-3.55993999214903
C	3.12850743425686	0.06757784625170	2.36417296341241
H	4.18223054900804	0.24872559592259	2.50772051645031
C	2.38972826510767	-1.01686584120739	2.88507594000468
H	2.76509490460098	-1.82076909277209	3.49932908965890
H	-2.02367455481827	-1.78271970934674	-3.22332448473881
H	-1.36554114859589	-0.15327861303676	-2.97536875701304
C	0.35315779903339	-3.07461304630303	3.25650524432024
H	-0.49780655318209	-3.75034884893131	3.35320765292828
H	0.77378541752513	-2.91993083094876	4.25102085469325
H	1.11210703206105	-3.56735803047882	2.64777167108451
C	-4.12319453575360	-1.52350271306487	-1.41926421433627
H	-4.54076034781312	-1.53840042639507	-0.41339017276902
C	-2.73720509955582	5.06068250850445	0.45917226085838
H	-2.35886490626151	5.81359939086602	1.15130019865174
H	-3.82111126787047	5.03308295891092	0.57538496926366
H	-2.50822243626507	5.38112583866609	-0.55699536201460
H	-3.98009865753901	-2.55538229621791	-1.74344757207792
H	-4.85521486643715	-1.06464120424297	-2.08561852267027
C	3.77520862279404	2.79719985513208	1.59937160131159
H	4.06431632058269	3.70852849512429	1.07542223908209
H	4.65550953499829	2.15369653347375	1.62148526385157
H	3.51105720864974	3.05561688484140	2.62369147886001
C	3.10870176006762	1.77368122770074	-0.54262284994230
H	2.30635760851847	1.45212981193635	-1.20046488181742
H	3.87497964338485	0.99446011556289	-0.51921015037029
H	3.54180362936379	2.66791927803610	-0.99532287968925
Al	-0.48183090171325	0.80459076353911	0.50114894217938
O	0.48638117844940	-0.17034655177948	-0.99658461523496
N	0.98848687415998	0.30423754700574	1.71933684976839
N	-2.14509282045269	1.41233018029304	-0.28435053957819
N	0.14591942151117	2.63097479336016	0.65690605619883
N	-1.35860441364483	-0.97178467843055	0.66908217952691
C	-0.63322744354060	3.76259622579950	0.65153984582042
C	-3.02817173985867	0.66158850605113	-1.02156862796166
C	1.70985476658056	-2.03115903823816	-1.78134294662249
C	-0.68318696772837	-1.97273713807081	1.28630508896198
C	1.44672054993295	3.05054644497515	0.80808259677071
C	-0.08766905424938	-1.74622697937225	2.64746149056302
C	-2.69899770206592	2.66223168922934	-0.16294711414328
C	2.60223049447739	-3.85474207015992	-3.63955226718032
C	1.09248150811951	-0.83674527730229	2.46966663506678
C	1.17957251745083	-2.02577428013968	-3.06915600519655
H	0.41552288720350	-1.30954393668999	-3.33191416428754
C	-1.12976668371539	-1.11332885663833	3.58462137177236
H	-1.48103419895554	-0.14885763543552	3.22028954396072
H	-0.69384747585140	-0.95302299909287	4.57231806306354
H	-2.00340795621743	-1.75998077754564	3.68782802983131
C	-3.89524671595572	2.71320915659982	-0.83408726827748
H	-4.55962465938670	3.55997994182930	-0.90397872078865
C	2.24864792611117	0.85875400160946	1.65851058693870
C	3.14770380333963	-3.87510439423754	-2.36373499843117
H	3.90835823034299	-4.59402417124406	-2.09936843879196
C	-1.84709094763601	-1.48675211372624	-0.51632588403516
C	0.15920228945804	4.87737165763850	0.75512014042834
H	-0.17269399463692	5.90294516384482	0.79156716648359
C	-1.43786635256749	-2.79198234935634	-0.65685033324830
H	-1.68205117809122	-3.45999333592729	-1.46944147329502
C	1.49105396131332	4.42169612656523	0.85186870456706
H	2.37121273345932	5.03633756331828	0.95601725644118
C	1.28699654595125	-1.07625617041453	-0.75885334986088
H	1.76575014809837	-1.17229716357955	0.21795150354425
C	-0.67227428780409	-3.10535535843644	0.48677233473445
H	-0.23855006628700	-4.06345564277946	0.73073847595843
N	3.07418971504207	-4.82121481105916	-4.62670454977094
O	3.92721625625168	-5.60340734724235	-4.28182980728540
O	2.58530989870009	-4.78103674115924	-5.72974366083030



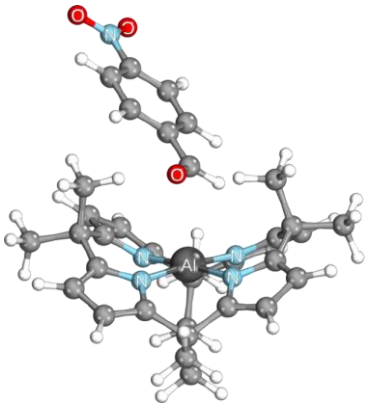
[**1**$^-$]-*p*-nitrobenzaldehyde 1,2 adduct B

Al	2.05288443891557	8.03447137832504	12.56299029502551
O	3.10220857842838	7.94460043535024	11.10362009455740
N	3.74340007120641	7.42781255914101	13.48591724144851
N	0.26472024629624	8.51402130712124	12.12244247456553
N	2.55335980954108	9.82534313035970	13.14772343999843
N	1.42776544335572	6.21369991065191	12.99228652776870
C	1.72509169608838	10.90391056767101	13.00857846531321
C	-0.63427080268121	7.67921714329519	11.50997428107092
C	4.90078355406789	6.40537309936777	10.77546647782356
C	1.95350897072894	5.28246975109347	13.84992588011946
C	3.83906463473478	10.27829802512750	12.95370112377582
C	2.99610906185899	5.63000996998409	14.88817267454148
C	-0.36735003940852	9.70609388061808	12.35198062814055
C	5.81857323776213	3.90411123735151	10.00188731819382
C	4.06918810653533	6.40548392810153	14.18191679364268
C	4.09119251261189	5.28226901069884	10.91947384490604
H	3.09418359421527	5.37271575824336	11.32728912917139
C	2.39659641242191	6.51761371825024	15.99463975518303
H	1.96456273512290	7.43233450266631	15.59054333469516
H	3.15129242222147	6.80105445385488	16.73313688549360
H	1.60219377126267	5.97188387208295	16.50401139821525
C	-1.65032577625961	9.64394705404808	11.86295940565520
H	-2.39654085556693	10.42226714307079	11.90706565420161
C	4.87531767154614	7.95676825228574	12.78098138278978
C	6.63265588511120	5.01275878417190	9.81478575452815
H	7.61114842642584	4.90972141886306	9.36953826852229
C	0.48452104374085	5.57495597700132	12.23120285757157
C	2.46293883327949	12.03171029580098	12.73682671068772
H	2.08572943556483	13.02982422291845	12.57915029550031
C	0.42341417869621	4.24606427634046	12.59575526482543
H	-0.22282777984935	3.49073261614818	12.17738389219550
C	3.81583391389967	11.62919791996538	12.69551279009240
H	4.66593794694597	12.27054898972055	12.51758183986786
C	4.44306805610357	7.77275946340005	11.24906307160369
H	5.00861370537666	8.52004588660198	10.67061038177384
C	1.36312364888245	4.05909417650409	13.63200958778975
H	1.56300875095662	3.13858378928607	14.15891149203904
C	4.54886556585997	4.03064917525587	10.54691543928778
H	3.91327239127803	3.16782474605230	10.68257948968731
C	-0.28685616520130	6.26355138586497	11.12504519381386
C	0.24264040271967	10.77683153268209	13.22002418518485
C	6.16203266628251	6.25158952128395	10.20358934091248
H	6.78924318574543	7.12394236253573	10.05647408748628
C	-1.82015574569832	8.34850171798907	11.32265122373141
H	-2.71528509323947	7.96040048961968	10.86208957747486
C	5.99101546672378	7.06965675681889	13.23005025322707
H	7.02032097294934	7.16337283908073	12.91744124659072
C	5.50349927583106	6.15235617003911	14.07599729923995
H	6.04185657082989	5.35181434185409	14.55886619659069
C	-1.57994428428698	5.48453556862701	10.86676527806207
H	-2.20652871615302	5.44280982395765	11.75725920482236
H	-1.36020690737522	4.46418585065918	10.55001930437311
H	-2.15154522781426	5.95136480717316	10.06386976227012
C	5.07747540408040	9.44945397502403	13.19975256939368
C	-0.01490566435065	10.41268426939278	14.69855249316746
H	0.42796371201235	9.44905877086895	14.95214477470416
H	-1.08698047392160	10.34263404987142	14.89213213592517
H	0.41695628433526	11.16409494197509	15.36404517981073
C	0.52093859490849	6.24238485829957	9.80975455541562
H	-0.06983452159257	6.68855538449809	9.00684675002576
H	0.76431882803971	5.21424193917280	9.52954214385014
H	1.45117297282694	6.80059265018330	9.88176819576868
C	3.57163695488494	4.36859315987104	15.52534412779974
H	2.78675109858883	3.81549719307784	16.03996102850881
H	4.33496005028033	4.61669172588794	16.26577336419522
H	4.01265324968482	3.70553879353329	14.78039443271477
C	-0.43560053420242	12.11729030047237	12.94123075859753
H	-0.02707420934265	12.89821819112851	13.58482621514933
H	-1.50561514055854	12.05647160474690	13.14149302383433
H	-0.30188571450665	12.41940628088779	11.90261194058718
C	5.39892913330301	9.51422570472084	14.70550614845012
H	5.49285614136112	10.55977734855561	14.99813234772521
H	6.33206544589735	9.00498852556280	14.95864335588354
H	4.59710244727429	9.08552275936502	15.30550535410171
C	6.27127822820549	10.04031798601798	12.44452236673530
H	6.08472479832920	10.12819119894171	11.37523548880226
H	7.17578524103397	9.44666439073589	12.59275262197572
H	6.48868121825611	11.04141034187866	12.81555419785179
N	6.30671483989755	2.59208090162854	9.60933815106259
O	5.58070913219741	1.64181403997937	9.78118441524206
O	7.41758358448649	2.52068973874534	9.13380016667207



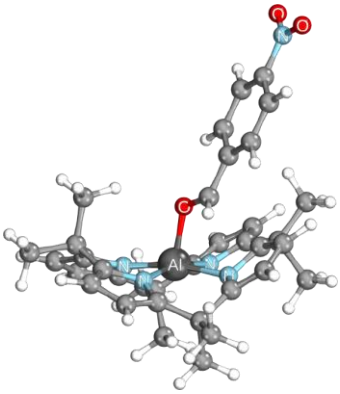
[**1**$^-$]-*p*-nitrobenzaldehyde 1,2 adduct A

N	-0.05511853538871	-2.32104099522403	0.40662879917814
C	-0.26376094622566	-3.50676284278696	1.05852860172639
C	0.37942028106982	-2.63001644382257	-0.85691451403074
C	0.03985800602046	-4.55640482741329	0.21905849373782
H	-0.02987574043392	-5.60785220854128	0.44843734433749
C	0.45071717407049	-3.99504193064386	-1.00819695235767
H	0.76634631139754	-4.53488901075223	-1.88801206580330
N	0.02514471760252	-1.25598910990756	2.92721750916042
C	0.62737792204898	-0.58706617012607	3.95885039082202
C	-0.20982924649459	-2.54003170291173	3.34831696259373
C	0.74934560584665	-1.42712845824885	5.03920728883703
C	0.21188317068975	-2.67564990475467	4.64924922898128
H	0.15789911476371	-3.56607351681229	5.25612778546080
N	0.03373587787876	1.27279537496150	1.63343680862148
C	-0.68113975523107	2.31451908778498	1.08172207730486
C	0.37550294145066	1.65714385064066	2.90104112162187
C	-0.79143455327283	3.33580944300305	1.99543487654946
H	-1.28374097378470	4.28500940649039	1.84740194835794
C	-0.11017375197123	2.91747901102632	3.16029635420455
H	0.00729106461773	3.48087159458422	4.07258990923981
C	-0.27568434389726	-0.50733715020351	-1.82801000680539
C	-1.63572873706645	0.98512077600112	-0.85295059465253
H	-0.06164644871875	-2.64898961113911	-3.57662493173096
C	0.87370114441373	-2.18102668775672	-3.26950523094135
C	2.12755554085251	-0.94475766033210	-1.50509326685886
C	0.77173582671146	-1.57973829043583	-1.87040892957615
H	2.89974890016657	-1.71408890190721	-1.51962618934406
H	1.65083689912995	-2.94388845293430	-3.29608827394492
H	2.11223634061350	-0.50924877892923	-0.50649733706254
H	-2.66589887811941	-2.43185019828737	2.01217762539342
C	-2.37147305300296	-3.40204873532756	2.40485865376883
C	-0.56678374630379	-4.96816309269107	3.03632093490308
C	-0.83881396615702	-3.57862074335468	2.45465719512304
H	0.50148548733147	-5.17573169529760	3.09484451416688
H	-2.81925705800793	-4.17199775388924	1.77168288944449
H	-1.03711680739205	-5.74090114117181	2.42664872075767
H	3.08435923194466	1.59801162022133	2.95646992350091
C	2.61452915940962	0.62340063622319	3.10956956094396
C	1.43370846753161	1.44635807733493	5.13337294364442
C	1.22949122051087	0.78101951839172	3.77329679733856
H	2.09734722978165	0.84846783109051	5.75866377792089
H	2.53578589549190	0.13485162969633	2.13810611992927
H	0.48803780210836	1.56633803121325	5.66202630190189
C	-1.08256664799286	2.36974360379087	-0.36985950204364
C	-2.07944087691624	3.50568349160354	-0.62215363141136
C	0.18037432655011	2.71714670302527	-1.18844091643678
H	-2.39801636162875	3.53088518904574	-1.66565454664024
H	-0.02162079347327	2.79395268988669	-2.25992968931184
H	-2.96527548603269	3.45701143943304	0.00298259450030
H	0.98185314541104	1.99763348125098	-1.03386789861015
H	-1.59373677135212	4.46045681916311	-0.41928644540307
H	0.55221737447231	3.68306243193429	-0.84684232670561
H	2.40780374237377	-0.15783412826277	-2.21069311424909
H	1.14163653471137	-1.41946528577877	-4.00516058836673
H	-0.98890584950268	-5.05095708450682	4.03841872672460
H	-2.78828518696573	-3.49355959214993	3.41032432255444
H	1.89261997457112	2.42955974557763	5.01664501554773
H	3.26737434506906	0.01079552259987	3.73432005186368
H	1.19516596499125	-1.19106116367399	5.99318375693782
Al	-0.47406541026031	-0.57669409025668	1.21970276787951
C	-2.77452110007183	0.26073912017761	0.01872818843531
O	-2.24891915930634	-0.28288211937474	1.14769361901324
C	-1.93016343952070	0.93651199939010	-2.31450302796004
H	-2.68022576697585	1.53396133545701	-2.81176446567620
C	-1.11364487542897	0.04286402218102	-2.89166664902661
H	-1.08104165193035	-0.24352935907449	-3.93175299164423
N	-0.56550455528333	0.03691676777957	-0.70858074246113
H	-3.15236624009703	-0.52106170655950	-0.66724570446234
C	-3.94240500618886	1.16464654055624	0.32728795573083
C	-6.06662971883032	2.85338728429664	0.87987920215732
C	-4.08119342172092	1.72538443296151	1.59377741360723
C	-4.90479075414245	1.43664621945895	-0.64084153194684
C	-5.96560230523467	2.28271687308226	-0.38095461411323
C	-5.13685264659017	2.57463532043347	1.87236888593325
H	-3.34272402115874	1.50582253986185	2.35172616838658
H	-4.82770405467025	0.97209829537468	-1.61715164916783
H	-6.70459095898430	2.48973143762181	-1.14059443383489
H	-5.23076334590071	3.01811431634225	2.85276678970842
N	-7.17619041565729	3.74946703213662	1.16547730404248
O	-7.25326239720470	4.22031206276800	2.27544223332378
O	-7.96277598111416	3.97695893938628	0.27462030676143



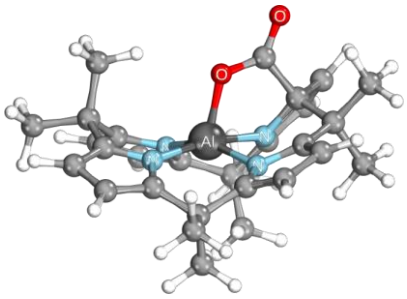
[**1**$^-$]-*p*-nitrobenzaldehyde TS 1 isomer B/A

C	2.49963984198075	2.42728875737425	0.80205523168573
C	-2.63280840812748	3.09054588107498	2.55301457538326
C	1.51337122187356	-3.91520715469234	-3.65557200390954
H	1.04043242005900	-4.13270096915146	-4.60164284447226
C	-2.59604509892806	-0.40731818224611	-1.71028714253460
C	-2.31807908494118	3.68764795027581	1.16302906192487
C	2.73620819133713	-3.38565157018348	-1.21715553967744
H	3.19638121066238	-3.16949257241007	-0.26019519449444
H	-2.15252128131843	2.12074469643031	2.70177990181671
C	-4.13333610823498	1.61495308563790	-1.30779904978326
H	-4.94954572764092	1.33572808901229	-1.95551689866658
H	-3.70762435581165	2.93999645435531	2.67162185203709
H	-2.27516365822083	3.75108787895326	3.34528619534691
C	-1.87349631729637	-0.10862940623168	-3.03962538438210
H	-2.54846402008571	0.42136607664691	-3.71408808761354
C	3.21470345392688	0.33070531059108	2.13852155281435
H	4.24890780064029	0.58426231847385	2.31017345721471
C	2.55724827768454	-0.84587758981958	2.56914856466887
H	2.98987539441601	-1.65787762568975	3.13303839011706
H	-1.55879439803029	-1.03502150500719	-3.52676739636359
H	-0.99426580427140	0.51335019276972	-2.89365508804229
C	0.66615399086292	-3.07835774808017	2.75222565665794
H	-0.14577072437607	-3.80050836693843	2.84737373206884
H	1.14307575739998	-2.98318562727627	3.72839767457092
H	1.40177785481261	-3.48354266543734	2.05626639925060
C	-3.86586773286986	-1.20341704101228	-2.05172276792098
H	-4.43514474125857	-1.43622148241564	-1.15297996903016
C	-3.03276544726687	5.03435767582410	1.06605270518118
H	-2.69293657618706	5.70853244746455	1.85301899706243
H	-4.10922056112922	4.91094101917638	1.18963966801166
H	-2.84934187639270	5.50951252889553	0.10274535295487
H	-3.61581346454277	-2.14053490853316	-2.54981688325897
H	-4.50806439412884	-0.64157664989303	-2.73102891755608
C	3.72415340028974	3.10674237838988	1.42020092545238
H	3.90686708961101	4.07221536532010	0.94739078647818
H	4.61965961128292	2.50288827585408	1.26732940922523
H	3.59330056796725	3.26546681992366	2.48999630220844
C	2.79044390327581	2.25343147011843	-0.70272711873070
H	1.93589059078216	1.85684358789348	-1.24478333239012
H	3.63240817479461	1.57502821793951	-0.85983585999814
H	3.03543444273016	3.22092438555600	-1.14550504904697
Al	-0.51305121762361	1.00673189352439	0.53603766517902
O	0.88468095658989	-0.32846300531989	-1.48965374534451
N	1.07552605451594	0.43692760550308	1.47279680331577
N	-2.17842813212670	1.58892867598582	-0.20728963066462
N	0.01369180600932	2.82167193851201	0.85101523808151
N	-1.13791031699653	-0.80658677872419	0.34997905800461
C	-0.83639282809616	3.88483133232976	1.04052740067297
C	-2.99421802399594	0.88916835538530	-1.06480470952072
C	1.84540650440488	-2.46962381965747	-1.76531106221217
C	-0.53353860182217	-1.87776515829545	0.94132196729388
C	1.29454913818951	3.30424040349086	0.98231907646856
C	0.13043947958337	-1.72922696245219	2.28099955006270
C	-2.83066793527708	2.75815533063315	0.10297208791406
C	2.40644570355274	-4.81679877345830	-3.08995230464693
C	1.25597619349604	-0.74580992703737	2.14265566922366
C	1.23768228422262	-2.73858532494112	-2.98813252152109
H	0.54036837622246	-2.02299533400214	-3.40075818731109
C	-0.89083134981413	-1.23638926138692	3.32360244349909
H	-1.31250858854766	-0.26407473231459	3.06580629399907
H	-0.41414345880982	-1.13385267358805	4.30014931407856
H	-1.72426013877900	-1.93621411884999	3.40959305218348
C	-4.03097500879525	2.80724961689062	-0.55751759435378
H	-4.76609029014871	3.59446910656428	-0.49930032103846
C	2.28336699420865	1.09621646049764	1.47743413850460
C	3.02559806956133	-4.56690574797005	-1.87385337331137
H	3.71544364594838	-5.28049200268269	-1.44898548951662
C	-1.74783363010214	-1.26082287661575	-0.79771647507779
C	-0.10845655543509	5.02406281044975	1.26632389073902
H	-0.50008425443497	6.00965052889442	1.46331445072438
C	-1.50270499481309	-2.60852215746538	-0.93691063788537
H	-1.85911082623333	-3.24914434885595	-1.72882882489415
C	1.25568903122246	4.65332158462997	1.22348991821195
H	2.10224429316530	5.30788632432609	1.35896562491195
C	1.58131101543404	-1.21060618665754	-1.03729368242086
H	2.09895652233116	-1.10819299642423	-0.07437901173556
C	-0.72350749898281	-3.00454045428829	0.17005343677175
H	-0.38531251898046	-4.00430951852567	0.39499292665196
N	2.70384298442694	-6.05867633825864	-3.79399525273743
O	3.48383806724775	-6.82451968554785	-3.27925817733341
O	2.15524563415144	-6.25100353823080	-4.85277086922709



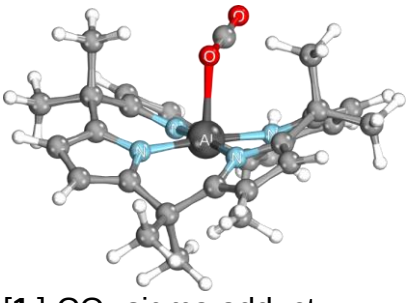
[**1**$^-$]-*p*-nitrobenzaldehyde TS 2 adduct A

C	2.73272368227292	2.14117503861886	1.40964474385111
C	-2.70813588635452	3.24628165053777	1.53162685580222
C	1.29468464271592	-1.56371660130523	-4.68738036421558
H	1.21860913327063	-0.95419481328325	-5.57549800824633
C	-2.30588407645474	-1.29287170174095	-1.17247998556628
C	-1.94647120467816	3.47992926107339	0.21016974453466
C	1.48828501373370	-3.15139807992460	-2.41423970138536
H	1.54679656450321	-3.76154659832693	-1.52164763972175
H	-2.36213110271213	2.34892148932749	2.04587768248302
C	-2.87650504322045	0.92829629838057	-2.31391290410544
H	-3.35668073734073	0.53428145378818	-3.19705838085091
H	-3.77797996505784	3.12649737318298	1.34607131197712
H	-2.55944961187701	4.08963387955703	2.20877626542419
C	-2.31498997592290	-1.99272096370137	-2.53186963599233
H	-3.18114249996023	-1.67903089578385	-3.11418645897190
C	3.02230171967944	0.38018082068369	3.26960199913623
H	3.98474925629600	0.69341733021820	3.64171226072060
C	2.25510526470838	-0.70230034724960	3.74805435825647
H	2.51324511177685	-1.36871556625354	4.55650676734750
H	-2.38681757987848	-3.07574145217749	-2.41881740101926
H	-1.42711096619398	-1.76989271981459	-3.11809334428323
C	0.29340825390003	-2.85098644073796	4.01411437746765
H	-0.55390356210970	-3.53358141872692	4.10150957124051
H	0.56474060706430	-2.53292680105364	5.02075213305690
H	1.13878079561000	-3.39975039602048	3.59832186647858
C	-3.65042804944836	-1.61120446969326	-0.47074702798920
H	-3.69251907667968	-1.13237969207678	0.50675977432735
C	-2.48803713320225	4.76158292375962	-0.41953206288707
H	-2.36520108289855	5.60668526172296	0.25872433393836
H	-3.55385369392794	4.66351236984985	-0.63206866642441
H	-1.97069063868310	4.99588475393081	-1.34986284190523
H	-3.77854817271603	-2.68786091459187	-0.33207079553213
H	-4.48160184392705	-1.23098790897519	-1.06698425212861
C	3.77421999830220	2.95198884745194	2.18940413103065
H	4.11214277160334	3.80606650265916	1.60192235283497
H	4.65556907184822	2.34612216147568	2.40313066006974
H	3.36989243489325	3.31950336118646	3.13184086523390
C	3.42724380496339	1.67349058298178	0.11270494567298
H	2.75668753787510	1.12819617251702	-0.54405715815919
H	4.27329560986452	1.02385570634179	0.34895328460419
H	3.79685498859525	2.53771305850121	-0.44345562705386
Al	-0.16847178684024	0.68714202584954	0.65615901047114
O	0.75261403077868	0.01455361416789	-0.87238315489923
N	1.12714130509970	0.28023034545532	2.06557638746104
N	-1.79242411104119	1.05843762330110	-0.34833376434124
N	0.31833315709421	2.54381688358408	0.75784450008242
N	-0.92265632194374	-1.18608669984828	0.89975075778790
C	-0.48003746217590	3.62855556112710	0.49797368501421
C	-2.24232315816279	0.20417349564478	-1.33283876195058
C	1.13084914259764	-1.80995485453591	-2.29969893459749
C	-0.50430249197517	-2.08887409803849	1.79130681003763
C	1.56042266336901	3.03008276055244	1.09160858093940
C	-0.07296030063268	-1.64456196254505	3.15379704761254
C	-2.18525711230673	2.31876467444734	-0.70831396557427
C	1.64544517769870	-2.90322968753653	-4.77759392142076
C	1.10840748671610	-0.72950185578573	2.99508426627589
C	1.04035828985735	-1.01807068951076	-3.44336857144442
H	0.75310085226418	0.02064146186305	-3.35091198648102
C	-1.23745566963562	-0.90319545977673	3.83843246850321
H	-1.54470406127550	-0.01988866944819	3.27915627754006
H	-0.92986829345027	-0.57244483291846	4.83138552689554
H	-2.11203060628801	-1.55021108393552	3.93962939932853
C	-2.84806324933137	2.28275712110532	-1.90986437472448
H	-3.27557194599947	3.12117117782251	-2.43707917011708
C	2.30692067468270	0.96289136765146	2.24928113951763
C	1.74850006979932	-3.70759104076440	-3.64966300141870
H	2.02529934006153	-4.74736332299467	-3.73815941222019
C	-1.23672204022773	-1.86068637159385	-0.26917220595413
C	0.24062160552007	4.78529815669784	0.65308111242176
H	-0.12212162733360	5.79311551917569	0.52355184412281
C	-1.00411582517541	-3.23206013733304	-0.05935495038606
H	-1.19573500896540	-4.02151863196396	-0.77079915472010
C	1.54695533459941	4.40213473186094	1.02984673060897
H	2.37362475745108	5.06487244906374	1.23197275810713
C	0.88262064292073	-1.23055806545657	-0.97138828052176
H	1.18482571955685	-1.83872619433943	-0.10999553012449
C	-0.52811155396065	-3.37742555390367	1.23587252339107
H	-0.22651630161455	-4.29119751042902	1.72292650099789
N	1.91485868512623	-3.48298031439417	-6.08737478873120
O	2.21347475863400	-4.65323539607725	-6.13306150347664
O	1.82490087427568	-2.76188505254937	-7.05183992306372



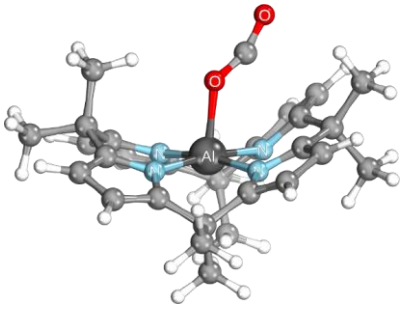
[**1**$^-$]-CO_2 1,2 adduct

Al	2.04134190655131	7.97566326269415	12.64814893291232
O	3.16384891833398	7.80164806481107	11.18496355569006
N	3.70292028373871	7.42792166888565	13.62204027524337
N	0.28734765726023	8.45806767913103	12.10984535739964
N	2.56228223339642	9.79140387666582	13.12664555486909
N	1.41172851227294	6.17679410357784	13.09894923860075
C	1.75249731937160	10.88149855878791	12.96334205287672
C	-0.59511322959727	7.61672917497564	11.48031667556493
C	1.86853866578825	5.29771522394219	14.04780507851178
C	3.86368690535879	10.24093203621875	13.04098114867131
C	2.94057405065299	5.65940180241715	15.05118249108720
C	-0.31705681026968	9.68221124633026	12.22443468073415
C	4.01341977020181	6.38588712566507	14.29708578111334
C	2.38198302563507	6.59768267240890	16.13788206613288
H	1.96079388007266	7.50654677690342	15.70976404536696
H	3.15640887544799	6.89155200032506	16.85160782319969
H	1.58667334619610	6.08617730946592	16.68026761166820
C	-1.56023722803817	9.63208447363821	11.64252766849749
H	-2.27993689419720	10.43415019754100	11.58696656558306
C	4.83314636243893	7.91088099043187	12.88225614763635
C	0.41021150478081	5.54272480606912	12.41316903757918
C	2.51543749017898	12.01034717221702	12.78158786489730
H	2.15706041687293	13.01603849002593	12.62865989775073
C	0.23193953774354	4.27600771772290	12.92421523250889
H	-0.47788378243292	3.53769697093346	12.58638329427120
C	3.86441471550819	11.59856401475519	12.82406661303837
H	4.72960339058612	12.23474809070537	12.71585965763780
C	4.43566128807719	7.81770487919449	11.37005675750011
C	1.16600993379577	4.11872955240404	13.97010424311462
H	1.29509618434433	3.24463529988481	14.59008934808356
C	-0.28170094298221	6.16453544175942	11.22152525169306
C	0.25852082536434	10.77295643092510	13.08939593687855
C	-1.73677134762354	8.31270259260542	11.16492995985742
H	-2.61012483860877	7.92655106380971	10.66288869302109
C	5.91363362117742	6.95183768532313	13.23857369251174
H	6.91464197789264	6.98991873955331	12.83770251006290
C	5.42259908489546	6.05615657882292	14.10744278105534
H	5.93772669406780	5.21781069240861	14.54995123765715
C	-1.58958125809068	5.41336752836590	10.95713677919454
H	-2.26198783306740	5.46715449432102	11.81301574914021
H	-1.39336807627094	4.36349160725551	10.73541616381487
H	-2.10109352172721	5.83278391905831	10.09022355940265
C	5.09075814465890	9.39627033760981	13.30428222906290
C	-0.08719005052330	10.45788339357112	14.56189975057529
H	0.33396141231782	9.50111209523722	14.87275183424436
H	-1.16912089090089	10.39901996397618	14.69543209909364
H	0.31097072869610	11.22889802974387	15.22582907662771
C	0.59088175523913	6.00674781206736	9.95838919675473
H	0.06781975325751	6.41930685388833	9.09294359770046
H	0.79460982425928	4.94994873954153	9.77066390693092
H	1.54597839284089	6.51911724919471	10.03860914927505
C	3.50162117569914	4.40937907058840	15.72384477330806
H	2.72001618668759	3.90157000105931	16.28773842034221
H	4.29594894819033	4.66653072936554	16.42792370620051
H	3.89694020853183	3.70194138276241	14.99453933857833
C	-0.38834758408237	12.11056891025847	12.73292236182231
H	-0.01270419442679	12.90582736016171	13.37864205521806
H	-1.46896383476805	12.06410165628555	12.87034163271751
H	-0.18807860922909	12.38276241707724	11.69674262698689
C	5.40851762897867	9.44566130934783	14.80929760143214
H	5.57403398833920	10.48401396579433	15.09614866499166
H	6.30646395263605	8.87701003942951	15.06371801253117
H	4.57977884506981	9.07551082739872	15.41153784530490
C	6.29782768215916	9.95512639006938	12.54707358891936
H	6.12705134965714	10.00620855432384	11.47505968591819
H	7.18988251999666	9.35123850278105	12.72316922226947
H	6.52040777732887	10.96087586535858	12.90295324316754
O	5.29801727428891	7.76948753017017	10.52778736799563



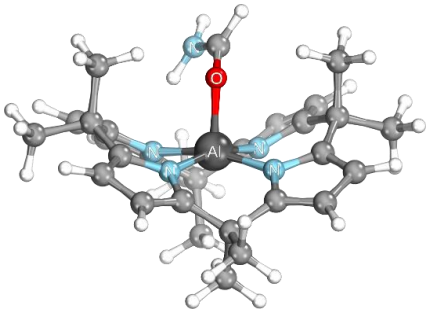
[**1**$^-$]-CO_2 sigma adduct

N	-2.39943790183754	-3.31258252916980	1.32639633808967
C	-1.06391807174690	-3.62859033597498	1.20809863631838
C	-3.09722878087994	-4.49327964580036	1.25629756240062
C	-0.93176623519829	-4.98400854347332	1.03055505671453
H	-0.01057099315264	-5.52907833369504	0.89668548272292
C	-2.22978261901829	-5.53728897801890	1.06688439726766
H	-2.48587634655347	-6.58206500150294	0.98744235168269
N	-1.54900531810407	-0.99059073576063	2.38502326747901
C	-1.42422602415876	0.06488826129265	3.25182557456051
C	-0.27370032318592	-1.41842839423134	2.07989355357670
C	-0.09811225034004	0.33307778727880	3.47424009535868
C	0.63523463607978	-0.60844997438287	2.72048368267815
H	1.71013431045005	-0.69271568690394	2.68063130481071
N	-4.01058254924548	0.15102605529562	1.85355891258924
C	-4.96640060697101	0.75888401026022	1.06664644249835
C	-3.60355500268496	1.07605161282319	2.78073811626124
C	-5.12074772078597	2.06300359283906	1.47647869859473
H	-5.79813307039959	2.79150934766608	1.05878248977215
C	-4.25691690177150	2.26374070071258	2.57468348526815
H	-4.14441024739166	3.16980259292687	3.14910279445610
N	-4.86044078143679	-2.17308841049956	0.80212224050920
C	-5.30042855603740	-3.47414189206507	0.79740742393935
C	-5.83967366084032	-1.41727942516255	0.19569752324478
C	-6.52048157767446	-3.55222327356465	0.17811468700960
H	-7.11602253379867	-4.44029908902709	0.03633651073184
C	-6.86202803383322	-2.23907375291935	-0.21087889847202
H	-7.76200375517175	-1.94097362122702	-0.72540599605232
H	-4.42617575150765	-3.40138773221514	3.41537869494358
C	-4.79733482762092	-4.36413042866401	3.05792037203753
C	-5.12145831660202	-5.92027757259867	1.15709411359822
C	-4.56789743775110	-4.54973571864852	1.54161820926945
H	-4.61823303103278	-6.70958115640756	1.71678025610304
H	-4.27699229557917	-5.14017224607491	3.62284360845142
H	-4.98984721926546	-6.11576077397962	0.09301111329681
H	1.12810350739800	-3.59397719473144	2.85292308659512
C	1.30372639143426	-3.28902466866820	1.82268333931571
C	0.43109687622265	-2.22434656659797	-0.22239595656843
C	0.05447089867597	-2.62007296902741	1.22331340679801
H	-0.42739455369187	-1.89739116342751	-0.80190965929711
H	1.59063459104921	-4.16842733855653	1.24572685718668
H	0.84836229045459	-3.08748518186521	-0.74499788326014
H	-3.10330632941608	2.40875371339551	5.11371327096627
C	-2.22990837625861	1.94497657845684	4.65322709589041
C	-3.30375333297438	-0.27972297088401	4.84646534324335
C	-2.63542857919925	0.70335808520865	3.86378474229358
H	-2.60725402162116	-0.56264748131407	5.63813519728765
H	-1.74835771351608	2.68342830991351	4.01208746350197
H	-3.62670437152991	-1.20055808659567	4.35766834519010
C	-5.75054858271385	0.06927483066263	-0.02615348895329
C	-7.17491200748059	0.65044467635986	-0.01253326964655
C	-5.18197891164490	0.36219619626777	-1.43319184888581
H	-7.79234538656549	0.18880896014146	-0.78339414358573
H	-5.88515357884861	0.01805698481401	-2.19435971892166
H	-7.65262109114383	0.49385381940152	0.95313162637886
H	-4.24597242844335	-0.15561417470142	-1.62162695724434
H	-7.15945326536041	1.72095954158199	-0.21970334848959
H	-5.02283205081763	1.43432533294257	-1.57124035631458
H	-6.18495567990721	-5.98558865814535	1.38982841950960
H	-5.86276768695868	-4.40611917686786	3.29284972485992
H	1.17805072728493	-1.42691840075370	-0.22404739630933
H	2.15556505275771	-2.60838536748495	1.80544150211317
H	-4.18879616879750	0.17248908803850	5.29825637144443
H	-1.53648817347911	1.68145623620663	5.45301963302764
H	0.30600744654322	1.10378373633179	4.11160290368837
Al	-3.17653638008033	-1.56536165714499	1.50022293548173
O	-2.31409908148095	-0.54815201504296	-0.30300925049766
C	-1.87294127399872	0.51335779765601	-0.08440739611841
O	-1.41779396084384	1.55415247530288	0.05310130760926



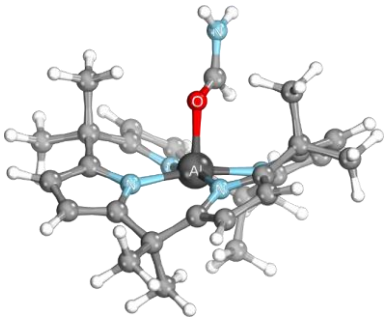
[**1**$^-$]-CO_2 TS2

Al	2.04547067937461	7.97719844903252	12.93469776851523
O	3.12015513422547	7.69336212851700	11.22480958264378
N	3.70638791302723	7.51676348547603	13.89292589456298
N	0.31671862893983	8.45450164175423	12.23205933310728
N	2.57823551250190	9.83641063449352	13.10430601392948
N	1.42890499241528	6.14045085588050	13.12922862797532
C	1.75076556084097	10.91388369310217	12.93012858764834
C	-0.53158513142333	7.63992717117237	11.51493043287126
C	1.85961652383456	5.20520923732807	14.03819265625519
C	3.86710103895308	10.29597907030494	12.94552674153518
C	2.88838471378799	5.52853744485457	15.08330167947214
C	-0.28996862615405	9.68444300934846	12.31346598611149
C	3.98160113808087	6.31561306230368	14.43103203048914
C	2.26036430789933	6.36084270297381	16.21797271886933
H	1.82732189742495	7.29274168721052	15.85389983533188
H	3.00656008075973	6.62059979433224	16.97237740556792
H	1.46054301277957	5.79363419305902	16.69663818857955
C	-1.48539792467178	9.66207869318652	11.64386337079089
H	-2.18403501551903	10.47808261629006	11.54523124492388
C	4.88093432092773	8.01531213018162	13.34878876849357
C	0.46035727155533	5.52932631262457	12.36484602549334
C	2.48735747794502	12.03400568527448	12.63846670126845
H	2.10681997715996	13.02576467641545	12.45117919085688
C	0.29362006502855	4.23158578429383	12.78501288741442
H	-0.38963602739733	3.50494799968607	12.37503076414353
C	3.84202295404754	11.63565234000661	12.63989049509346
H	4.69865664612877	12.27215928350541	12.47568638377678
C	4.28770766415060	7.53906260261576	11.06497067332719
C	1.18680172298337	4.02478409922165	13.85744935715974
H	1.31202454009326	3.11728729953384	14.42745730973645
C	-0.24106013151635	6.19526401759714	11.20975340823148
C	0.27581841627346	10.78785172207788	13.15705708302074
C	-1.63750072852639	8.35609535808776	11.12950174215390
H	-2.47300618153222	7.99030533050457	10.55387916324958
C	5.88500945837203	7.06596870933819	13.55243997381695
H	6.92179390077945	7.17191904637093	13.26928980683528
C	5.31920762894171	5.99136964194838	14.23986762447702
H	5.81097063776057	5.08019390124655	14.54112522785742
C	-1.56788749487795	5.46840669739380	10.95494125375693
H	-2.21672209952687	5.50799331700686	11.82885679829045
H	-1.39289270580714	4.42266549129745	10.69974460756597
H	-2.09566681764590	5.91484718882787	10.11188310021558
C	5.09954926916167	9.51230709492187	13.31114432929056
C	0.01359568610330	10.47928554018123	14.64681878798227
H	0.47471137837589	9.54052418987862	14.95764461874506
H	-1.05836394246519	10.39227809000256	14.83467274411432
H	0.42164933685442	11.26876611558164	15.28176242736890
C	0.58112803361219	6.05918150594661	9.91073307800137
H	0.02987225288929	6.49112154089013	9.07273127644292
H	0.77683954571027	5.00653780648912	9.69497255931565
H	1.53678183577651	6.56990404941538	9.96721989678650
C	3.45038437342091	4.24698328656898	15.69313961669262
H	2.66663064054197	3.69280945686254	16.21036252610776
H	4.22837987017705	4.47816393212755	16.42299326271470
H	3.87492950577859	3.59409182999122	14.93054356040047
C	-0.41799743253372	12.10783954244258	12.82888578434973
H	-0.01680603870149	12.91459266794347	13.44412928354447
H	-1.48757507808229	12.04217199898837	13.03151997974203
H	-0.28553197439531	12.37552723526048	11.78061512383797
C	5.48728964157243	9.92026741159399	14.75450080465446
H	5.64425015607853	10.98555512582302	14.81724813247514
H	6.40006303379819	9.41078108171024	15.07248392648182
H	4.69054972472637	9.65612874085542	15.44930574597422
C	6.26507192280666	9.89014712711988	12.39247061821665
H	6.03428162422989	9.73555280944714	11.34022370263674
H	7.16215489903422	9.31717239478701	12.63230018448149
H	6.51820441451711	10.94323619069560	12.51684549321220
O	5.26005938861781	7.33058002879714	10.47267809101250



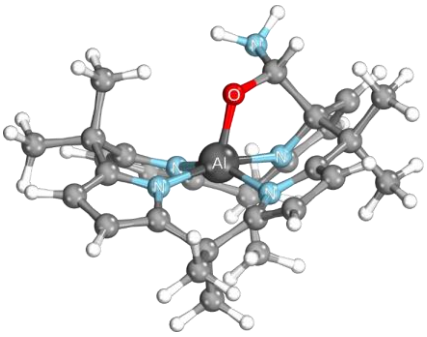
[**1**$^-$]-formamide sigma adduct isomer B

C	2.38163153880223	1.55864890471670	1.06676543327647
C	-3.48811410861692	-1.14484470499599	0.07693315472836
C	-1.84657730000037	3.50683220839615	-0.81324773066145
C	-4.14542678734606	0.71284373839658	-1.57959637035134
H	-4.98756232622593	0.22607504234333	-2.04656996041059
C	-2.71654474605256	-2.20971271715206	-0.73208007545662
H	-2.76023164982416	-3.18210875612518	-0.23517947480873
C	2.34917728152091	0.39935187733320	3.37282954877792
H	3.41598622570435	0.30801335301615	3.51390225846737
C	1.35234575581371	0.09213710786748	4.32454707989550
H	1.50623792111975	-0.29538198228521	5.32025316302573
H	-1.67463963755205	-1.93889263558842	-0.87179410024307
H	-3.15814369844618	-2.30901894385574	-1.72583824710480
C	-1.20344830885821	-0.24400342295398	5.71521028353430
H	-2.20765570327339	-0.29259610420920	6.13860801690765
H	-0.59105113029768	0.37016880682729	6.37672313838579
H	-0.78864193176423	-1.25298513014424	5.71174655309229
C	-4.96856083853543	-1.55947206071347	0.04209638650498
H	-5.58554277396261	-0.85872920949715	0.60245476979774
C	-2.07965338511857	4.46014704737438	-1.98437049155249
H	-1.58021730428477	5.41403469663422	-1.81077007331109
H	-3.14313184660453	4.66962497638509	-2.10569066730858
H	-1.70332366485032	4.04001797375706	-2.91701184104675
H	-5.10608581920690	-2.55491434855448	0.46632352329937
H	-5.33658411065882	-1.59932368986498	-0.98343247207999
C	3.55692215852013	2.40010075186551	1.59860366004026
H	4.08808810528136	2.89284422465132	0.78360191797280
H	4.28152229644009	1.77234729755344	2.11896713239439
H	3.20582693182830	3.16275321503166	2.29175268041830
C	2.99298869951216	0.51090117709126	0.10987230484032
H	2.23029433869123	0.00275568245886	-0.47480978346829
H	3.58031724427887	-0.22991925786647	0.65991795460844
H	3.65423411667294	1.00558981841044	-0.60429769273898
N	0.35365676978044	0.91383163282293	2.48668215034286
N	-2.38033068371654	1.12153478117532	-0.25601613888810
N	0.10010923290239	2.28542048966805	0.18839963943982
N	-2.18284033368535	-0.21218305144041	2.06956403845980
C	-0.37507485594757	3.27804012355860	-0.62643676088648
C	-3.35502804289315	0.20715499297288	-0.57412342654238
C	-2.07810250251229	-0.49688629433926	3.40569054044630
C	1.45777658079212	2.46568639519772	0.29470265755820
C	-1.23900846372350	0.35675597633315	4.31295312408581
C	-2.58780549100842	2.22201003855600	-1.04512823663086
C	0.15002517834651	0.43290976657067	3.74744626693353
C	-1.84528638917919	1.76800509353474	4.41825309033549
H	-1.90298751638036	2.26364997409140	3.44947641955260
H	-1.23609870432348	2.39768821638935	5.06974559825337
H	-2.85866818123942	1.71955354996465	4.82211025624307
C	-3.65738952930177	2.00265560625940	-1.87824137645086
H	-4.06535532901309	2.69188385519319	-2.60096460026196
C	1.70885456693895	0.92709245520186	2.26907650373277
C	-3.05166356160517	-1.12537529133959	1.52508468439050
C	0.66388723213712	4.06801640199804	-1.05451790639899
H	0.59649393767148	4.93320640469676	-1.69539682565861
C	-3.45993185562017	-2.00579954046483	2.50531609079110
H	-4.14549978037188	-2.83030216754758	2.38567604674917
C	1.83595208283789	3.54621174384552	-0.46828874928538
H	2.83718689905924	3.92761109812036	-0.59710815376967
C	0.55432778615977	-1.60021162030766	0.86530071680095
C	-2.83807924268141	-1.60612779108800	3.70826146913931
H	-2.96810028134432	-2.05219274832313	4.68248242649694
Al	-0.92259379349465	0.84903388926705	0.98014476694319
O	-0.00681044220572	-0.68086266795700	0.24716790247397
C	-2.41138340107240	4.18075591402289	0.45731233880144
H	-1.90090915158831	5.12694090735522	0.64950105421327
H	-2.27883132129378	3.55340812147186	1.34023935119807
H	-3.48171686093866	4.36895014364191	0.34893598608530
H	1.47906052334809	-2.01572804291219	0.45540649896375
N	0.13273860260694	-2.18684159040276	1.95879712114877
H	-0.66914983716392	-1.84929624300494	2.49110339641652
H	0.75510261701734	-2.81426645908582	2.43473505935208



[**1**$^-$]-formamide sigma adduct isomer A

C	2.38456459650542	1.55920020664223	1.03417462584677
C	-3.45553274185325	-1.13399776330940	0.02348726679979
C	-1.83859084173926	3.54069322727801	-0.81085808390228
C	-4.15156313339933	0.75656614947667	-1.57722652896733
H	-4.99461792847791	0.27139853944785	-2.04439134827992
C	-2.71890562547591	-2.16363814152297	-0.86239148693468
H	-2.72241113668880	-3.15209825794619	-0.39572537740432
C	2.36144129611416	0.46404990971555	3.36718584255158
H	3.42889118519183	0.38378910211453	3.50836725952940
C	1.36656117301069	0.12765284961730	4.31137103303793
H	1.52368090190290	-0.26498838164800	5.30435953094428
H	-1.69014446389940	-1.87198444363128	-1.05475468447325
H	-3.21485357572030	-2.23827612023676	-1.83253754226644
C	-1.18186061550882	-0.31617581208761	5.67726591875624
H	-2.18816790260081	-0.41326790566756	6.08740141398618
H	-0.60159406992288	0.30872088747047	6.35781325537414
H	-0.72756148574149	-1.30747568360641	5.65688825571280
C	-4.93783319486840	-1.54789881823727	0.02998916470678
H	-5.52873263451605	-0.86831872787221	0.64194745364969
C	-2.08014043982154	4.50242479337162	-1.97320631626246
H	-1.56908818534124	5.45066516678469	-1.80198522258870
H	-3.14340720120808	4.72209286259569	-2.07752430573428
H	-1.72180715054932	4.08375954434081	-2.91358331067273
H	-5.05945944468692	-2.55745516272494	0.42449605236423
H	-5.34904672660009	-1.54897844812355	-0.98013824188076
C	3.59003028109637	2.38532311565578	1.51724932196629
H	4.12376671222276	2.82942172916965	0.67618060156724
H	4.30377480546618	1.75776444686485	2.05241389512806
H	3.27118845249250	3.18490606955888	2.18396159112093
C	2.95100817364322	0.45937814617730	0.10839819028320
H	2.16328936200207	-0.08118253536641	-0.40922424479576
H	3.55424961144455	-0.25491338047010	0.67477742315947
H	3.58260761073380	0.91191251430491	-0.65902246049377
N	0.35855237421626	0.93652225019633	2.47249833716206
N	-2.37490419654546	1.15377864619910	-0.26664553888853
N	0.10844961908032	2.30087123445242	0.16530317980545
N	-2.15788210145636	-0.22504878620956	2.03658329912334
C	-0.36665076705102	3.29402184299442	-0.64924186799402
C	-3.34769409204336	0.23894772129179	-0.58806041689575
C	-2.02796901924669	-0.55801961296269	3.35614786467941
C	1.46936604580375	2.46492683389600	0.25160999485902
C	-1.22908549053632	0.30871210695268	4.28604469509306
C	-2.59322914624836	2.26320658941426	-1.03946368066257
C	0.15943863586510	0.44020016155028	3.73050497689723
C	-1.88373446911770	1.69633715727106	4.41304065583051
H	-1.95293583767903	2.20840353903353	3.45339739868744
H	-1.30170586696506	2.33447510075824	5.08119767309562
H	-2.89786412286883	1.60576872115321	4.80759339172263
C	-3.67193745882529	2.05249366445216	-1.86301834189752
H	-4.08880180748623	2.74991429998570	-2.57279188555870
C	1.71548349675444	0.97575167010594	2.26085835258958
C	-2.96780721648971	-1.17135001607278	1.45644679991501
C	0.67607113950560	4.06634867491749	-1.09939166348075
H	0.60994829082503	4.92802390621454	-1.74521397365456
C	-3.30896342008325	-2.11632001509574	2.40155442705806
H	-3.95115123311487	-2.97143584738809	2.25311493619321
C	1.85037684860789	3.53349306672815	-0.52658164007781
H	2.85416931144432	3.90241208961748	-0.67052893688454
C	0.25149643202143	-1.61846568581594	1.01417501198856
C	-2.71345671233231	-1.72091443771027	3.61939637068319
H	-2.80499564836774	-2.21519775539097	4.57447888724304
Al	-0.92279243399113	0.88383295019330	0.97715757467937
O	-0.06120303312686	-0.70041056748944	0.24700044779670
C	-2.37534224746030	4.21398233208412	0.47199596462794
H	-1.85119281164396	5.15328173672214	0.66104359109436
H	-2.23607851053847	3.58111303752183	1.35002889566241
H	-3.44503555975038	4.41479990002540	0.38162864633893
H	0.06301123221374	-1.57911251304224	2.09236157344068
N	0.83854940272585	-2.72139572052432	0.57971808085483
H	1.08463902398686	-3.45043636765913	1.22266097169766
H	1.04950568671148	-2.84048158650651	-0.39735294465291



[**1**$^-$]-formamide 1,2 adduct isomer B

N	-0.11234781266972	-2.28130280317041	0.40125825645214
C	-0.42604510967756	-3.43359982515670	1.06885526026885
C	0.41955529215243	-2.64681995290331	-0.80619638149839
C	-0.09437412512652	-4.52266863968508	0.29168201881412
H	-0.22459805375520	-5.56266281491203	0.54697053331154
C	0.44874362881895	-4.01840368597728	-0.90943158169418
H	0.81978860333164	-4.59922359972277	-1.74031214271165
N	-0.18079149619369	-1.13054551899052	2.86763219423316
C	0.40105522486594	-0.45099764931826	3.90313025084888
C	-0.49272548494051	-2.38600254993711	3.31974242455032
C	0.42855859651452	-1.25431090773083	5.01876748580565
C	-0.14582374011932	-2.49161818076136	4.64608988042597
H	-0.26980343220494	-3.35646254608262	5.27941676223482
N	-0.02835867476072	1.33868027004785	1.51413649296365
C	-0.66803471803623	2.38604720198330	0.89548029532040
C	0.33279964421490	1.76749943109432	2.75929804373548
C	-0.69908135368798	3.46929206546950	1.74444128810839
H	-1.11958401732015	4.44248364293510	1.53822121709383
C	-0.05277644923672	3.07562414585342	2.93676727845538
H	0.09795602343988	3.68190300108972	3.81633437937556
C	-0.04044868065767	-0.52189976283701	-1.89625120693072
C	-1.47617335191264	0.99205085916903	-1.09905623427936
H	0.22910356407534	-2.72676067310334	-3.55161739606522
C	1.15512987761600	-2.29454995749112	-3.17169756257064
C	2.29700485982674	-1.06346241802578	-1.32923037182445
C	0.95153854886362	-1.64415734610800	-1.80586675407362
H	3.02733174171553	-1.86839834335439	-1.24266411798329
H	1.89277240575833	-3.09352774133574	-3.10409710070111
H	2.20644348995786	-0.58961857472475	-0.35255765564833
H	-2.84822680389552	-2.22100477574524	1.85195310243220
C	-2.62064934452133	-3.20107800304089	2.26424281213218
C	-0.92780223645185	-4.80959417258893	3.06740279215471
C	-1.10286904273636	-3.43275742240564	2.42173055045694
H	0.12495823780166	-5.05645437004522	3.20237313685650
H	-3.05190508862135	-3.95938045339000	1.60528860026121
H	-1.38914295740860	-5.58489021211703	2.45376504916147
H	3.02935169409920	1.53841066002027	2.93276827175451
C	2.49166058300785	0.60165964136288	3.09897559776007
C	1.28537546521927	1.57360062099967	5.03947879614925
C	1.09346097850758	0.87222327848444	3.69595146320906
H	1.88235411722963	0.95889512926636	5.71398001738780
H	2.42040008091499	0.08412770658240	2.14190425137497
H	0.32820765576904	1.77471391901998	5.52056376511051
C	-1.10542413420933	2.40303345176430	-0.55343499479431
C	-2.29681195118658	3.35083192436725	-0.72794479395892
C	0.06819875981400	2.95871534427240	-1.38467470215985
H	-2.66874350529802	3.34747760326950	-1.75549395286593
H	-0.19711392229836	3.11223676953833	-2.43408182209994
H	-3.11928628209549	3.09985264492902	-0.06054805327069
H	0.93149595140169	2.29451604343805	-1.34308708687130
H	-1.99915782971682	4.37532378601810	-0.50474670756019
H	0.37820748370112	3.91702845453363	-0.96811289537307
H	2.68346042525003	-0.31699948898571	-2.02879641039135
H	1.52738986935732	-1.56978330784086	-3.89916745572877
H	-1.41615176272187	-4.83852147289736	4.04229301065278
H	-3.11002385273490	-3.26916579015913	3.23862444804174
H	1.81210263812506	2.52034129734016	4.90785049932798
H	3.07799967400592	-0.02899920044268	3.77033955006196
H	0.83787198798306	-1.00287744403259	5.98524078905920
Al	-0.55020788155650	-0.49533787653962	1.10192946389512
C	-2.70352926921948	0.27726787392892	-0.35145083622518
O	-2.30542622250163	-0.15090408035981	0.87153714446424
C	-1.60018091668560	0.93705363488110	-2.58141598183392
H	-2.28760386131903	1.53180017423376	-3.16648864436295
C	-0.73955416083246	0.02581761326933	-3.05362185138034
H	-0.60468004427442	-0.28574062056749	-4.07803424585416
N	-0.41350912018867	0.07025643154097	-0.82630382106108
H	-3.50713184967213	1.02956155815490	-0.26311585983538
N	-3.12493518779381	-0.85612069660196	-1.15912214757721
H	-3.46268974356751	-1.57659298716540	-0.53671334405138
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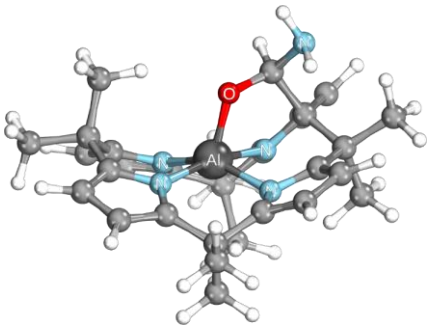
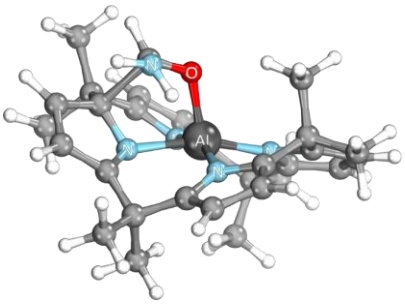


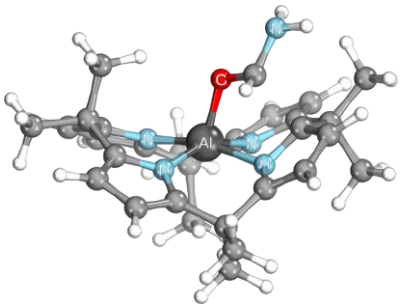
[**1**$^-$]-formamide 1,2 adduct isomer A

N	-0.06110927569263	-2.30861188915900	0.37232918740926
C	-0.30029619638952	-3.47684037101050	1.04344469697501
C	0.44129984125975	-2.65073660554303	-0.85691895917465
C	0.05601608069110	-4.54875963251892	0.25360823891435
H	-0.02162582173970	-5.59380833465797	0.50893498564950
C	0.53040328778521	-4.01935288127146	-0.96450553877954
H	0.89570122010757	-4.58124926734828	-1.81079099065933
N	-0.16424392329521	-1.16850173162657	2.86537063733364
C	0.34500532118236	-0.46399832187719	3.92252924368071
C	-0.41586847389720	-2.44328081459293	3.30344119254438
C	0.39345825626078	-1.27292610308909	5.03262140108272
C	-0.09552158053914	-2.53868018073421	4.63692307630540
H	-0.18583106465759	-3.41365395657213	5.26173868667482
N	-0.07923918901343	1.33468700348896	1.51235876466059
C	-0.72006197344210	2.37098565524723	0.86755708245915
C	0.15809256083415	1.75510959363241	2.79147428998880
C	-0.89761169124229	3.42106880624846	1.73779481149397
H	-1.34908513355753	4.37608590235973	1.51469449121108
C	-0.32931310246485	3.02856052951833	2.97110775163780
H	-0.28296826371123	3.61814373503244	3.87322300491341
C	-0.17414959596586	-0.55602810911208	-1.92173715694334
C	-1.55566522292076	0.98261742000626	-1.05792657428593
H	0.11031341025361	-2.75186024382498	-3.59120991244211
C	1.03271941634285	-2.27390280228797	-3.26016627319192
C	2.21261573280891	-0.98452826869111	-1.48324009172321
C	0.87261711058684	-1.63039009527301	-1.88527626196332
H	2.98589316672663	-1.75242767652868	-1.44949771867751
H	1.81012260445138	-3.03657930352239	-3.23290971404714
H	2.15567930844604	-0.52754340028390	-0.49591359586715
H	-2.76724972012961	-2.40299250529495	1.79130200347255
C	-2.49472986136300	-3.35730695684432	2.23587655238491
C	-0.72373704082985	-4.88358823270833	3.03916897447782
C	-0.96755550741415	-3.51481704298677	2.39856193919138
H	0.33979361089308	-5.07659297075829	3.17847833405066
H	-2.88899276104784	-4.15167561634834	1.59706444683403
H	-1.14222178894350	-5.67899442038051	2.42091781505010
H	2.84812461290914	1.72918325782938	3.06701295136248
C	2.37864259387878	0.75226832200199	3.20671613494228
C	1.02895092411972	1.60680581569287	5.10836458054367
C	0.94266068579092	0.90765289973452	3.75259373577747
H	1.64448447493540	1.03101527502758	5.80005074356364
H	2.38210152924880	0.23954745906358	2.24470867850220
H	0.04188709818513	1.72888815393456	5.55433350713801
C	-0.96967611081543	2.36990352264602	-0.61829409392482
C	-1.87904880795987	3.52280086927036	-1.05538737804575
C	0.38882762309130	2.61159752668819	-1.30998878353224
H	-1.90802172760860	3.58709263663964	-2.14530921757113
H	0.32012473763721	2.55327032995814	-2.39936819369706
H	-2.90058749905720	3.42123557182410	-0.70300879153209
H	1.15444496858079	1.91846027305483	-0.96902019527793
H	-1.47282564374916	4.46854768156356	-0.69632492951176
H	0.72896103948515	3.61461986684462	-1.04975288945036
H	2.51922399277506	-0.21278197212197	-2.19463932384793
H	1.33001640110260	-1.53371139642376	-4.00629173253959
H	-1.21469737247660	-4.94240117190340	4.01124345988439
H	-2.98054249711867	-3.42253982303918	3.21227540890188
H	1.48732855129109	2.59190161496817	5.00608631036741
H	2.98602935749328	0.16341038316275	3.89687361065938
H	0.76016325449520	-1.00472988517012	6.01152811140236
Al	-0.55930450304207	-0.53837177379856	1.10498073453749
C	-2.77188285784100	0.38747582468414	-0.21060036279818
O	-2.31558494250074	-0.28224741356758	0.89295098702562
C	-1.79386642522274	0.88373113678814	-2.52513031392028
H	-2.53722581667966	1.45790997937853	-3.05807553599825
C	-0.95966062224539	-0.03190228044878	-3.03947581153151
H	-0.88852119730807	-0.35721411189329	-4.06624078730941
N	-0.51327077419423	0.01910722741266	-0.83352848126483
H	-3.26948762366001	-0.31375293004982	-0.90101498264231
N	-3.74616771577770	1.40970125768742	0.08618381461073
H	-4.56018501391083	0.94800353187432	0.47378130346173
H	-3.37388843422480	1.97656242999941	0.84357391107371



[**1**$^-$]-formamide TS2 isomer B

N	-0.16987802279416	-2.26191593859245	0.38595839741533
C	-0.55365336407633	-3.39432190386946	1.05793521224365
C	0.33450724274939	-2.66357188373554	-0.82499071998181
C	-0.30746928038705	-4.49974451422145	0.27306993733499
H	-0.50610639108559	-5.52872919763460	0.52807019478533
C	0.26039861600170	-4.03260351850385	-0.93188206993946
H	0.59039207652509	-4.63580514673745	-1.76405218643886
N	-0.16034060011355	-1.09873189741933	2.84664364183235
C	0.43553322118739	-0.43178543179198	3.88387324175515
C	-0.52782982696805	-2.33681398602189	3.30751290490398
C	0.42407153805666	-1.22661035955273	5.00479662344157
C	-0.19421994993909	-2.44389774960402	4.63692658272628
H	-0.35931675950231	-3.29609320293863	5.27776688337757
N	-0.03986294967737	1.37170874647806	1.54440206000946
C	-0.64821136623810	2.43594909342711	0.93009758003834
C	0.38803847908853	1.79667041421051	2.76932884305656
C	-0.59889900505412	3.53045407654986	1.76436378118337
H	-0.98196133125980	4.51889840188152	1.55470279708366
C	0.07003539913084	3.12341211033809	2.93977426667040
H	0.28328678082780	3.73470862414298	3.80283052299569
C	0.03411928842947	-0.50977581555770	-1.91689156100518
C	-1.29203629849478	1.08680321707855	-1.16377132400148
H	0.20295511184216	-2.73541688092590	-3.56834654966251
C	1.14244014788788	-2.35334368484739	-3.16740753272742
C	2.32185335716974	-1.21593442727780	-1.29558681077646
C	0.94878699782394	-1.69380929926072	-1.80466816301020
H	2.99189367812939	-2.07036644891691	-1.19346791587098
H	1.83530964481646	-3.19084082885210	-3.08899081543633
H	2.24717499482277	-0.73585238853384	-0.32068875029274
H	-2.92512022314692	-2.11820340719585	1.87244064466122
C	-2.70947683787826	-3.08927083441611	2.30947987244645
C	-1.04529626858122	-4.74390761618356	3.07410375726673
C	-1.19538304148027	-3.36360374739842	2.42697676498894
H	0.00237040953504	-5.02228925616131	3.18477789471507
H	-3.18404958932684	-3.85173344819349	1.68656824927305
H	-1.54602413120480	-5.50759413737443	2.47722029867750
H	3.08723320099520	1.51577287986886	2.88784363056155
C	2.53387749749332	0.58766469034855	3.04976436040302
C	1.38682890259125	1.55918916068175	5.02498602036529
C	1.15337656136667	0.87739114132426	3.67826852424952
H	1.98465685798354	0.92524706624279	5.68081323019244
H	2.43575859271141	0.08855571442066	2.08498032971704
H	0.44381281124183	1.77559509973416	5.52685331211649
C	-1.17737333443907	2.46352793522048	-0.48935732621680
C	-2.53010569298144	3.18443648408929	-0.52360755748418
C	-0.16962953094054	3.28379958844286	-1.32532543873083
H	-2.97782396455986	3.15998718452091	-1.52148505380345
H	-0.52627340828620	3.45325918192453	-2.34485318542027
H	-3.23333032374243	2.75208920979310	0.18621674687920
H	0.78877925532834	2.76651272326996	-1.38147166206164
H	-2.40780778938263	4.23373787256344	-0.25468935111293
H	0.00624412482286	4.25322971670523	-0.85826430844814
H	2.77301708623653	-0.49811640252231	-1.98524484684435
H	1.56345697921441	-1.64627982875138	-3.88504315958952
H	-1.51087904499750	-4.75425203235551	4.06021929635836
H	-3.16809441754114	-3.11661883967430	3.30043362929354
H	1.93040081408621	2.49608899250598	4.89227298505957
H	3.12028080306015	-0.06612927047993	3.69865866838868
H	0.83109821555404	-0.98160573606025	5.97376284004346
Al	-0.49541838687253	-0.44509523338111	1.08342025318121
C	-2.68312243026447	0.04991378627439	-0.40553253746996
O	-2.27957891417478	-0.14354689781714	0.83137503043923
C	-1.44521298881441	1.02267980858606	-2.59622512450606
H	-2.10355638932779	1.64788105542612	-3.18328560321108
C	-0.66044895321908	0.01109361033838	-3.05863725432844
H	-0.58649595200296	-0.35687838447975	-4.07060365466534
N	-0.28169173553730	0.16333665433559	-0.84752099342352
H	-3.50775760621326	0.75929754732568	-0.53223184603651
N	-2.91013849358610	-1.11192297555177	-1.13565552218551
H	-2.26364188436206	-1.86692848508225	-0.94547591364221
H	-3.06036420825580	-0.98501575017506	-2.12240207180710



[**1**$^-$]-formamide TS2 isomer A

C	2.47224127276106	1.79739669887793	1.20677372275113
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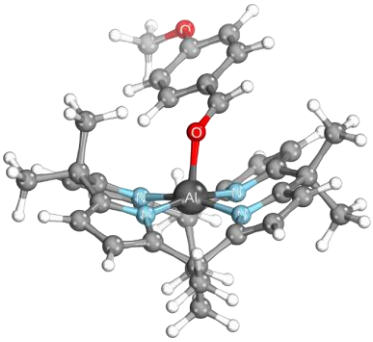
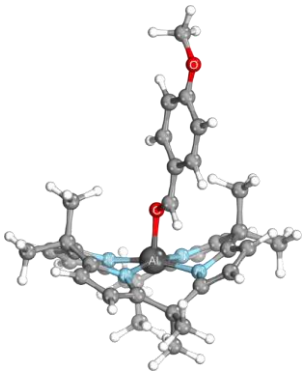
C	-1.75459823630022	3.45300012609422	-0.90761224413119
C	-3.53034774104723	0.34497618828170	-1.87822361682701
H	-4.16898518073661	-0.28926407147895	-2.47528758206176
C	-3.58088147156249	-2.38290035644375	-0.72974885565308
H	-3.77982740356193	-3.28465248149445	-0.14632029499084
C	2.32520450017851	1.27584564773926	3.73560524200967
H	3.33776167020297	1.51822112478731	4.01713896115493
C	1.31383972563827	0.79113801013586	4.59140244505041
H	1.40181700165960	0.60238097420733	5.65048410164858
H	-2.76127791389368	-2.58725299214525	-1.41457901784895
H	-4.46706023747492	-2.20148450400354	-1.33794253666201
C	-1.11454621839158	-0.45641919328842	5.64525624686686
H	-2.10407239109001	-0.79130321030075	5.96343039514870
H	-0.75818181296979	0.25914164725558	6.38596162606275
H	-0.43809259570344	-1.31146489913533	5.65593814029048
C	-4.61510116149406	-0.86208703799718	0.93239710037751
H	-4.47377682391209	-0.01928418634667	1.60824258341576
C	-1.99819837100782	4.34661993930145	-2.12213419264690
H	-1.60166164152604	5.34788038952749	-1.95016921275802
H	-3.06731099428325	4.44656516128791	-2.31721741692411
H	-1.52069353835491	3.94095416337701	-3.01406333791645
H	-4.95813015650093	-1.71865021341969	1.51930077330367
H	-5.39856521127534	-0.58915549764813	0.22379765122097
C	3.72168295857918	2.60582302749197	1.57025153506691
H	4.25523988359020	2.90943015835344	0.66882375190394
H	4.41257996223221	2.00349008361599	2.16165621308056
H	3.46816025132338	3.50021905601191	2.13870684798401
C	2.95720323851891	0.56049120349377	0.42154596470955
H	2.13703235590442	-0.07428030965728	0.09843976112279
H	3.62543527708525	-0.04161718738963	1.04218290008514
H	3.50293783824827	0.87741908301964	-0.47020279816608
N	0.46238807724363	0.97472292713141	2.51672385161518
N	-2.25113589477635	1.11532679673734	-0.19916788670212
N	0.23725037148524	2.37037171627352	0.17654943883627
N	-1.84985449817825	-0.40033537456177	2.00839849192205
C	-0.27810485067363	3.34256856205660	-0.63976691778513
C	-2.97367208662216	0.03850716699547	-0.65785175727892
C	-1.72115510032747	-0.77100718411210	3.25463181587450
C	1.56863144352533	2.65123482104758	0.35544022990271
C	-1.17811028863459	0.19367990950503	4.26563695982661
C	-2.36892288212308	2.10279679933885	-1.13653675581513
C	0.19403309434067	0.62099447812025	3.81353936129953
C	-2.12127690095745	1.40969915547945	4.34470086078549
H	-2.20027539426928	1.92281804663765	3.38689475192205
H	-1.73460556880368	2.12484137788990	5.07169280901927
H	-3.12887207164380	1.11329022985295	4.64760420814038
C	-3.14815222177792	1.67083878820492	-2.18270832716268
H	-3.41680972698639	2.23206450317007	-3.06402070664665
C	1.77323573769302	1.37794795663138	2.47816459477182
C	-2.25517089906095	-1.50453562283940	1.23750480079889
C	0.71566800185271	4.22134792418475	-0.99501888015046
H	0.61156860105156	5.09436612568168	-1.62077876985981
C	-2.48698906646086	-2.57101613172290	2.17368221551105
H	-2.85935739063704	-3.55573321886398	1.92744826240863
C	1.89801063241967	3.77714144175760	-0.36070576150996
H	2.86974945151210	4.24186672193358	-0.42172683140177
C	-0.46561991528654	-1.80751416939373	0.56703708206932
C	-2.11504981200104	-2.13560908810113	3.41213985685558
H	-2.09114936773561	-2.70284064134674	4.32962309336988
Al	-0.67186593994166	0.85295279178222	0.91522989472962
O	-0.10359038664218	-0.66486591690334	0.05785321816561
C	-2.43649428894845	4.11413812261882	0.30925517897819
H	-2.01888571802395	5.10733597126322	0.48634044976544
H	-2.28855139690153	3.52958695213450	1.21782180423896
H	-3.51307030147369	4.20657245968799	0.14680373693831
H	-0.07363054517061	-2.07207719528922	1.56154254451881
N	-0.37090263144027	-2.87371565571069	-0.32017165617447
H	-0.81321475670942	-3.72134019821778	-0.00598546632131
H	-0.64443213103367	-2.62836939604483	-1.25973582212825



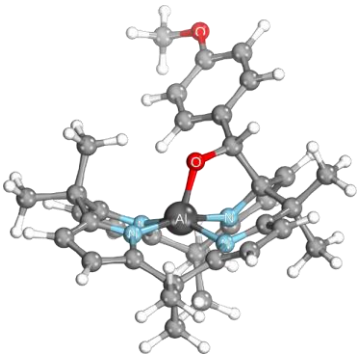
[**1**$^-$]-*p*-methoxybenzaldehyde sigma adduct isomer B

N	-0.48440417470434	-2.56743874034131	1.24291712479676
C	-1.06246483962723	-3.47320451933633	2.10435207173698
C	-0.02780484196532	-3.28249228427997	0.16707581877610
C	-0.97707450203502	-4.73853801117063	1.56588409683308
H	-1.33190521833681	-5.65320261965417	2.01414248962545
C	-0.30810821496551	-4.61774791575931	0.32978919731877
H	-0.05428209887761	-5.41785276993501	-0.34846045649022
N	-0.53466329931998	-0.86486079097831	3.35739817600189
C	0.01689603272516	-0.01482809353227	4.28227538881070
C	-1.02368677571072	-1.94306122154583	4.05779192325492
C	-0.13284144332286	-0.52935561551511	5.54510666274713
C	-0.80224532634557	-1.76268418192220	5.40159485957870
H	-1.07857976348757	-2.43619837816249	6.19751875183504
C	-0.11396094106269	-1.40583016538564	-1.40559728597815
C	-0.90403850173230	0.63744948681454	-1.21590780088274
H	-0.21702486370713	-3.93240897317761	-2.49278829442715
C	0.76664067089531	-3.59397940195269	-2.16390457417215
C	2.08536688343237	-2.20098986506435	-0.58841659291992
C	0.65766625314298	-2.62260529522143	-0.99100877984681
H	2.66919098063980	-3.07607045954128	-0.29828787172034
H	1.35356534171698	-4.47027474858005	-1.88609006593866
H	2.08106910247567	-1.51318660777561	0.25690756250223
H	-3.69316532834422	-2.62229788718347	4.18381913850233
C	-3.22229463576935	-2.80355348545107	3.21526212586769
C	-1.64661906891259	-4.31672271863747	4.35150577726645
C	-1.72109411409230	-3.10643584062033	3.41084083707240
H	-0.61476354252263	-4.60886080816666	4.54193142770354
H	-3.38889639477215	-1.92166614253102	2.60492988554391
H	-2.17615056434618	-5.17112079714357	3.92816638386759
H	1.50567473744181	3.03684978542701	4.78968792471758
C	0.95193651191785	2.14163598549762	5.07718791410290
C	2.18196462176595	0.80782652513506	3.38725967795024
C	0.77554305565832	1.21333925163724	3.87740525375184
H	2.75212754342532	1.68723049461083	3.07905470312883
H	1.51615057724289	1.64711918220125	5.86876583079701
H	2.13383309313929	0.13282914517138	2.53202169036173
C	-0.86782371608674	2.06811519215174	-0.74326127060175
C	-2.07404312016852	2.85396375601829	-1.26985105079025
C	0.40571108710747	2.68739286092273	-1.37607151899150
H	-3.00588421005113	2.53179384977857	-0.80553619832908
H	0.51322059921883	3.73272152630386	-1.08064356534595
H	-1.96383886108796	3.91834498655668	-1.06074950460066
H	0.37132532405676	2.62665917988858	-2.46625309818952
H	-2.17648896392218	2.74788441092034	-2.35105137689075
H	1.28965440222441	2.14889524389344	-1.03515848907728
H	2.59036808796219	-1.70008671939080	-1.41723751212369
H	1.26469132978294	-3.11714901898294	-3.00945315508775
H	-2.12433196818024	-4.09183930703518	5.30547197140667
H	-3.72469446071334	-3.64873937590498	2.73777000395832
H	2.72730653112267	0.29305927739145	4.18096053109524
H	-0.01073746400812	2.44807595217895	5.48655183452355
H	0.20880880176566	-0.08486383991774	6.46682630137614
C	-1.11051918277142	0.24107006734816	-2.52833495072267
H	-1.52992810705868	0.84374232563378	-3.32064091154826
C	-0.60461237054463	-1.06034360636543	-2.65270705957971
H	-0.60143484282920	-1.67269711804004	-3.54057421600519
N	-0.31207934264494	-0.39202930908374	-0.52325053006847
C	0.05939130177200	1.93078206081482	2.77582954698685
C	-0.30909501425555	3.25068803686541	2.70091492483264
H	-0.20887771073199	3.99423452771782	3.47609680891403
C	-0.82712927842374	3.44812408144353	1.40229439795559
H	-1.16857924824878	4.38343149179236	0.98346995643837
C	-0.73491809908369	2.24308823596493	0.74598103230689
N	-0.21585764815420	1.29346185953100	1.59619457877862
C	-3.15910674633802	-0.26909797112271	0.06820503114138
Al	-0.62671521363780	-0.60731854739501	1.43131917242944
O	-2.52227021556719	-0.39201653886790	1.12444019245769
H	-3.64870645692179	0.69390794520024	-0.12436737641434
C	-3.44164937584366	-1.31190092329044	-0.88019448305266
C	-3.97999574297421	-3.24783442737443	-2.80928117430035
C	-4.13816064310455	-0.97984221086872	-2.05134654461019
C	-3.03471734502740	-2.63088529286922	-0.69123513374072
C	-3.30563193814116	-3.59677611082193	-1.64647882624176
C	-4.40850860822618	-1.92558482929793	-3.00436670748805
H	-4.43744024377973	0.04836698261089	-2.21676097942122
H	-2.53773299144875	-2.93016717039973	0.21905391690908
H	-2.95757203744366	-4.60216488245492	-1.45649435602849
H	-4.93073485905079	-1.66874773319092	-3.91636778846594
O	-4.26845697323899	-4.10673610391563	-3.80163223904953
C	-3.79551997735871	-5.42604217087792	-3.69871475511805
H	-2.70549173477529	-5.46638852188740	-3.61343715634152
H	-4.09440772011069	-5.93460283885403	-4.61298063965800
H	-4.22970898471868	-5.95596680064743	-2.84557760570298



[**1**$^-$]-*p*-methoxybenzaldehyde sigma adduct isomer A

N	-1.20682540986015	-2.26110303489631	0.93850897740424
C	-2.18314638453504	-2.88763779220617	1.67255615175076
C	-1.17237863450927	-2.86445764487424	-0.28622194462892
C	-2.79730611438117	-3.84643393565676	0.8893341651338
H	-3.58206758818897	-4.52019111273975	1.20124924582551
C	-2.14233628150832	-3.84055008678130	-0.36209648340151
H	-2.33853666213680	-4.49294625200283	-1.19908952859193
N	-0.71239516630807	-0.77417688025601	3.12011493870751
C	0.05732422657212	-0.13117011768693	4.05259249950519
C	-1.43535384355005	-1.73288013033766	3.78689521805589
C	-0.18803619506952	-0.65036367078712	5.30020179340065
C	-1.14584051098460	-1.67165588619646	5.13043274599148
H	-1.56831904739577	-2.28837529677499	5.90921827854583
C	-0.42637507975514	-0.99158059556324	-1.65630721281374
C	-0.76221971593167	1.16285571205659	-1.31565329487508
H	-1.26139014776916	-3.21095783264726	-3.02185873479358
C	-0.27889039498553	-3.30129651416080	-2.55751329033309
C	1.25779289836842	-2.59193675059011	-0.74568757620786
C	-0.16650968725172	-2.42971547474865	-1.30948404324154
H	1.45372915217773	-3.63319381613811	-0.48038604019079
H	-0.11184685154114	-4.35036603311446	-2.30776673778700
H	1.41491543651138	-1.99328363733744	0.15157304430376
H	-4.07146303920106	-2.19892657080638	4.48876705099920
C	-3.86291059282198	-2.16585447468927	3.41773768585803
C	-2.29906041700987	-4.04646746143868	3.82776364979795
C	-2.42956198380742	-2.66778250525604	3.14843240974656
H	-1.30512168488215	-4.46114880167364	3.66615416406532
H	-3.99739430485636	-1.13366315990463	3.10278079502771
H	-3.03046444741895	-4.74896098985393	3.42553360006595
H	2.42680809853869	2.29005225382114	4.60661613703602
C	1.62987409697630	1.59754153518226	4.88034360672644
C	2.30770891734477	0.08463221733192	3.03705019980405
C	1.11558008706358	0.85294478409736	3.64963566517325
H	3.09887031846172	0.77653344980761	2.74048623672030
H	2.04346137933447	0.89882461270286	5.60869524528689
H	2.01559548733462	-0.47539425936859	2.14717763985536
C	-0.96333057331590	2.48404954084996	-0.60893127386415
C	-2.46067161503968	2.82001078657757	-0.42987398243424
C	-0.38407561333243	3.59368637726352	-1.50004406328317
H	-2.94617962952342	2.17154918846863	0.29244616603845
H	-0.50713660705745	4.57049425475394	-1.03149179323973
H	-2.56873522121558	3.84315693698759	-0.06278851896982
H	-0.90525961967927	3.63508557669357	-2.45731952217659
H	-2.99171644279281	2.73396951258241	-1.38079470256299
H	0.67590563384317	3.43310952757329	-1.69066795790195
H	1.99455001785924	-2.27245859567007	-1.48511950139653
H	0.46947354425333	-3.01198529009042	-3.29639087294124
H	-2.46973119636643	-3.97635218695739	4.90284504289134
H	-4.60522373663136	-2.78210666000288	2.90468102404380
H	2.71220463071856	-0.63213600070735	3.75497898213457
H	0.83276728287692	2.16402208388578	5.36180765703383
H	0.27737331848660	-0.35218163571491	6.22665263083118
C	-0.69982801923485	0.97194516872762	-2.67798121832368
H	-0.78133917632532	1.73189156012927	-3.43935482971424
C	-0.48124840212639	-0.40485191659962	-2.89631857522742
H	-0.36370204986088	-0.89691954999605	-3.84951426949353
N	-0.60819915289834	-0.04799967101412	-0.68031121519085
C	0.59694395589437	1.83263394428510	2.63822473850835
C	0.86597004381742	3.17533615730749	2.54512677219524
H	1.41408453313906	3.77460420760789	3.25532546357766
C	0.31812013691304	3.61361911652251	1.32021545720897
H	0.35748454933580	4.61749552488815	0.92702343549505
C	-0.25372137795799	2.51707164159144	0.71967001013846
N	-0.10503899615241	1.42040859962776	1.53530062705755
C	-3.50296190455055	-0.63058694595607	0.41185961111408
Al	-0.85390786100619	-0.33472917698582	1.24094676429682
O	-2.78364254002114	0.03123207687244	1.16228302312890
H	-3.07284803138388	-1.35055357730077	-0.29583513817334
C	-4.93971080605702	-0.45999696016869	0.37707895574253
C	-7.70784046869051	-0.20602844703294	0.26619592246464
C	-5.69632022800721	-1.31105469952572	-0.43142557563914
C	-5.58638706024869	0.51571250011746	1.13113738649114
C	-6.96006396917709	0.64988605499446	1.07838740379764
C	-7.06591202639625	-1.19099590782386	-0.48902500672955
H	-5.19179442569139	-2.08082207699979	-1.00296734088282
H	-5.00538019184056	1.17522158807735	1.76237948043311
H	-7.43312608069610	1.41909188603386	1.67248567654663
H	-7.65815404992096	-1.85054444764192	-1.10898984095781
O	-9.04396691774059	-0.15532464197336	0.15122656020830
C	-9.75272820110984	0.80726130168063	0.88988676093411
H	-9.62105126518462	0.67968586192089	1.96852450156906
H	-10.80434396517018	0.66731466619713	0.65007068897667
H	-9.46661211775787	1.82831189943207	0.62016119832188



[**1**$^-$]-*p*-methoxybenzaldehyde 1,2 adduct isomer B

N	-0.77802749474756	-2.77464952195449	0.82884415951673
C	-0.96407689610549	-3.90194283899606	1.58324350292665
C	-0.29672014221840	-3.17783013972069	-0.38901108502340
C	-0.61118195760677	-5.01278841126647	0.84532363705978
H	-0.64690975071346	-6.04104295687369	1.16922780557379
C	-0.18321082637045	-4.54889209570469	-0.41718834978015
H	0.17744304498872	-5.15319431881256	-1.23576133058697
N	-0.92622460436531	-1.43296417418724	3.19066988946906
C	-0.39819579935013	-0.59712653233506	4.13664283511100
C	-1.02791830158245	-2.68017043088402	3.75011802431474
C	-0.19348391398679	-1.29737072616114	5.30190560393656
C	-0.59829801340433	-2.62930954007998	5.05517156865172
H	-0.56308922340600	-3.44882527193260	5.75613228663501
C	-1.06104730702828	-1.23173081711353	-1.61435107506565
C	-2.65364461426277	0.15600461017172	-0.86850337142880
H	-0.55410985356851	-3.49806286221514	-3.11380110738224
C	0.32164195297781	-2.92880854225385	-2.80058939999146
C	1.34681238618744	-1.41655429180560	-1.10322029489960
C	0.07697757682198	-2.20166313924478	-1.48146939196287
H	2.17948577151881	-2.11062723645255	-0.98650310013419
H	1.15404132850479	-3.62451661583815	-2.69929000109810
H	1.22516021149215	-0.88209999886448	-0.16186191163224
H	-3.49675062572747	-3.88102241334212	3.93362072965633
C	-3.08817513878062	-3.84785166508404	2.92114734556017
C	-1.14393957326660	-5.15163565335314	3.71361028094435
C	-1.54599789370117	-3.86868769084939	2.98040074397332
H	-0.06094669634904	-5.24758526624955	3.78751157515258
H	-3.47661151768066	-2.95425834991351	2.43848403891411
H	-1.53492113332869	-6.03022172865918	3.19852524141974
H	0.56187913981395	2.62758056865725	4.84758579534527
C	0.19123818878562	1.62609330519249	5.07287565833759
C	1.48002542333587	0.69129642614989	3.16637270214562
C	0.07417446737418	0.79350963953218	3.79712603731336
H	1.85952042989579	1.68168977294157	2.90311423664536
H	0.89355768868015	1.16756938676385	5.76963757279235
H	1.46324490720783	0.08861920827764	2.25785918952573
C	-2.36745883443570	1.64738793850711	-0.49846771345344
C	-3.60901655373647	2.49678199580818	-0.78493824976725
C	-1.22311220345192	2.18131203917890	-1.38228215294222
H	-4.43796961300433	2.25608484442276	-0.12135565244522
H	-0.99935581200764	3.20587960488555	-1.08530667080388
H	-3.38015866293787	3.55309404565569	-0.64547439139735
H	-1.47861089002667	2.18268739314353	-2.44484920045228
H	-3.94585670330136	2.38075221236308	-1.81724817941668
H	-0.30970442315201	1.60284303970886	-1.24786574079159
H	1.60979994302092	-0.68513989596772	-1.87222971254112
H	0.58035158545058	-2.22401624076567	-3.59359656105577
H	-1.56081553473509	-5.16099844542971	4.72138312580762
H	-3.45889382345818	-4.71557252453284	2.36930119017681
H	2.17650870193403	0.21866612526432	3.86176020467256
H	-0.77218551811898	1.71842935358637	5.57411892571822
H	0.22360768623811	-0.91422577809093	6.22057255491533
C	-2.83009356984684	-0.05538333063962	-2.33620305648796
H	-3.61549564542902	0.38301075156400	-2.93346826257925
C	-1.86805501878600	-0.87673949969982	-2.77755746933100
H	-1.73230185226641	-1.25116745283473	-3.78014884676707
N	-1.48612025198168	-0.62468661333992	-0.57248190808732
C	-0.83966010575834	1.48234769935039	2.82314871031905
C	-1.41739726306680	2.72659891925480	2.91581177980507
H	-1.34696854748676	3.41289566412199	3.74508923340401
C	-2.13166839938602	2.93004847814248	1.71462240296002
H	-2.69529905848961	3.81201539378294	1.44958754888866
C	-1.94694390058418	1.80535954701894	0.94407843451067
N	-1.15062201548563	0.91022891140519	1.62161269476499
C	-3.77612393506105	-0.53787772838972	0.04275310885033
Al	-1.44683287289200	-1.00634005006007	1.40546876201032
H	-4.54776544813392	0.22737020680204	0.22112144429518
O	-3.23002102412021	-0.96849549811306	1.21608671120538
C	-4.43138994534596	-1.65974811991611	-0.74069187054405
C	-5.58993530270887	-3.68126251458071	-2.30786682030553
C	-5.55071700405972	-1.40999987555303	-1.53053277716374
C	-3.92337999539040	-2.94957780606336	-0.72988315821122
C	-4.48563945527370	-3.95307809610902	-1.50981414790436
C	-6.12845007690218	-2.39659464067870	-2.30761139832671
H	-5.98614513729813	-0.41556155209763	-1.53646861921322
H	-3.07392344838129	-3.19836076414878	-0.10890512608394
H	-4.03931347761962	-4.93762247438358	-1.46759919877493
H	-7.00349210337393	-2.18755486391219	-2.91030929448750
O	-6.20877328975690	-4.59290705785261	-3.10071542553418
C	-5.71064205501177	-5.90071754645450	-3.10487612535127
H	-4.67496910534877	-5.95384791458573	-3.45804237775168
H	-6.33707656571826	-6.47307117301272	-3.78750852570529
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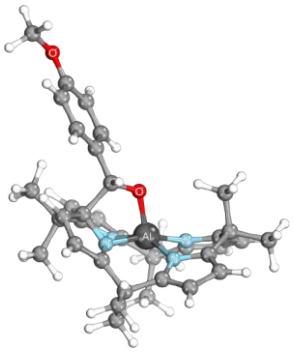
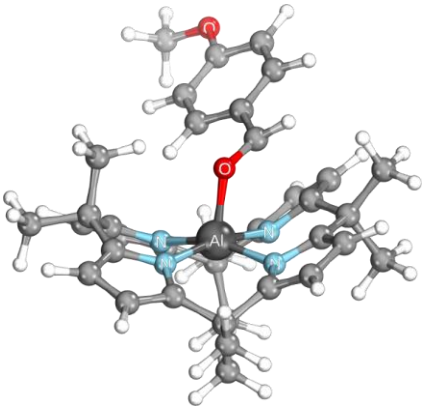


[**1**$^-$]-*p*-methoxybenzaldehyde 1,2 adduct isomer A

N	-0.71723008867919	-2.70186690493098	0.78907408655278
C	-0.89685563095837	-3.84805832594626	1.51509855701315
C	-0.22547581177418	-3.07610724400964	-0.43477432135514
C	-0.51823716943233	-4.93823229219458	0.76170823245174
H	-0.55029020320399	-5.97354546023561	1.06232386400479
C	-0.08832108198066	-4.44381449697967	-0.48763913632416
H	0.28157800939375	-5.02727785431313	-1.31716509191886
N	-0.76496351628277	-1.46458406913322	3.22950928600650
C	-0.21917546021292	-0.70204345388531	4.22644452306921
C	-0.95561068171802	-2.72611078533983	3.73143291477044
C	-0.08945376091539	-1.46143210106485	5.36459178709668
C	-0.56279005613318	-2.75581387212171	5.04840125837508
H	-0.59443765814801	-3.60556977544933	5.71254235633178
C	-0.93473853628732	-1.05312016505976	-1.57176641241662
C	-2.39674792795108	0.43229929524291	-0.74456053794790
H	-0.57318673960238	-3.29963681433381	-3.15850365230036
C	0.33112420950313	-2.77072309617949	-2.85607251680984
C	1.47215127550548	-1.36477658998532	-1.14333580599103
C	0.15649787374312	-2.08046114813764	-1.50590395032791
H	2.27498802165534	-2.09945885685753	-1.07766990493487
H	1.13987622332838	-3.49887237584535	-2.80615298573635
H	1.40341507012643	-0.86105621706155	-0.17975398844604
H	-3.49563613372388	-3.78162197819390	3.78418096694438
C	-3.05038139079051	-3.73998693756266	2.78751054155311
C	-1.20647347978483	-5.18266100282612	3.57971580565037
C	-1.51454599011481	-3.84884818282979	2.89481948093086
H	-0.13320297939728	-5.34128896427066	3.68323784741642
H	-3.37071045797258	-2.81137827511955	2.32112777943842
H	-1.62643074412964	-6.01404752383218	3.01176330849663
H	0.88607581630075	2.43198386705073	5.10777495782383
C	0.46604835467602	1.43942571331320	5.27940886252800
C	1.73743281967043	0.53554071532190	3.34675568826184
C	0.32877640160272	0.67636061869399	3.96298893179753
H	2.16909913953518	1.51761118214757	3.13837260468472
H	1.13577994073966	0.91434454341749	5.96117038214690
H	1.70569256973974	-0.02021026317340	2.40939058184183
C	-1.93678177287384	1.87277309830496	-0.33523083531136
C	-2.98770037731474	2.93125994590616	-0.68575958337344
C	-0.67087004478447	2.23904433139641	-1.14140741157595
H	-3.88917885284273	2.86532536413179	-0.08521784167921
H	-0.35921294465683	3.24267662152244	-0.85170637800713
H	-2.56227873589622	3.92354874968203	-0.53120032087207
H	-0.84702965496513	2.23919977894066	-2.22029029329372
H	-3.27382127880381	2.87176602288774	-1.73738511035323
H	0.16226377447263	1.57349679700843	-0.92386710850485
H	1.74487107253484	-0.61778937084358	-1.89397828766873
H	0.59116729770789	-2.04951029109294	-3.63403462848193
H	-1.65641787151998	-5.21374064316364	4.57271371644050
H	-3.44623621621394	-4.56877897505627	2.19523550115692
H	2.39855613986520	-0.00413942285109	4.02771318542064
H	-0.49889600302663	1.55297670261465	5.77345834626772
H	0.32083982942164	-1.14207373010037	6.31032483147242
C	-2.63386746436437	0.27486074170506	-2.20727926627942
H	-3.39690910227011	0.79782649124077	-2.76492551660596
C	-1.75815503424426	-0.61618058130279	-2.69644532664423
H	-1.67871200460787	-0.97254254476285	-3.71220409729224
N	-1.28584728251165	-0.44718321469148	-0.50264165974465
C	-0.53621440973814	1.45365787878767	3.01157648399250
C	-1.07755619549895	2.70792952758566	3.16875037753888
H	-1.00705957337737	3.33815292469781	4.04146236212276
C	-1.74547114153324	3.01357840201018	1.96144306777787
H	-2.27486397300610	3.92655853886296	1.73485020244120
C	-1.57189535025031	1.93548328489384	1.12645004344789
N	-0.82931277214538	0.96708147091079	1.76741210114697
C	-3.53573689104657	-0.29675596210278	0.12688924037173
Al	-1.24772634806244	-0.92469500373912	1.46408203596316
O	-3.02526540029601	-0.72121240526126	1.31664003334585
H	-3.82125011567759	-1.15205816435495	-0.51402608675650
C	-4.77317678506428	0.54628447165418	0.31321296086619
C	-7.04158816199740	2.16042769699763	0.63635630681691
C	-5.00864131421588	1.21017839947692	1.51609548230580
C	-5.70630772721219	0.68088939138217	-0.70018833222289
C	-6.83317906488252	1.48408204192736	-0.55923113858383
C	-6.12339106724818	2.01008148157124	1.67444719570421
H	-4.29585126966144	1.10734439313486	2.32260844107955
H	-5.56464220183893	0.14427541066758	-1.63256154813600
H	-7.53164581480376	1.55658757009700	-1.38229291096027
H	-6.29479406843113	2.53023870836963	2.60841053676296
O	-8.10219489552894	2.96966086576507	0.88357416830034
C	-9.04855541590202	3.14318465020642	-0.12982293975568
H	-8.61814346457955	3.58776702655613	-1.03450449666873
H	-9.80534128272871	3.82263667443648	0.25921534658350
H	-9.53973999470521	2.20461794567548	-0.41101914923244



[**1**$^-$]-*p*-methoxybenzaldehyde TS2 isomer B

N	-0.88848726621878	-2.81103441164593	0.86750692055786
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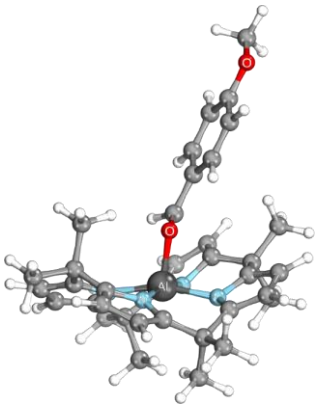
C	-0.51904448453076	-3.30295835760382	-0.35657417433270
C	-0.90039361675920	-5.05684802598111	0.96904130857825
H	-0.99310658716409	-6.06565276844836	1.33919152223231
C	-0.51321641549596	-4.67689968964191	-0.33351616656222
H	-0.25208739678815	-5.33639609758434	-1.14685296111023
N	-0.85492607615456	-1.37865640403970	3.17974410236607
C	-0.28491946230866	-0.53528890830833	4.09792192454529
C	-1.00256102615585	-2.59826818424938	3.79469534625834
C	-0.09171027344259	-1.19805262914122	5.28425410025151
C	-0.55407667401526	-2.51798771383727	5.09106313202245
H	-0.54669780605611	-3.31127235289089	5.82202103011119
C	-1.23937145801094	-1.34068705381862	-1.62695112081460
C	-2.46776305105963	0.36578361268222	-0.97948831662206
H	-1.06336493702742	-3.71959899291198	-3.01393483960374
C	-0.12012131162217	-3.21124269413849	-2.81041653079879
C	1.17807698665315	-1.72866725896446	-1.29410567758549
C	-0.18929015647601	-2.40599852040425	-1.51535343201340
H	1.95925385527567	-2.48703645514854	-1.22211484223277
H	0.66561590360318	-3.96473831132809	-2.75142920230188
H	1.19663829662730	-1.14698707212153	-0.37292349334733
H	-3.47024272476997	-3.74617197469165	4.20833781847756
C	-3.13961165956790	-3.75156755915023	3.16738207153902
C	-1.17004686756954	-5.06322986045592	3.86021336813553
C	-1.59763998445679	-3.79695212362740	3.10822533572666
H	-0.08694460261745	-5.18020611596603	3.86002805626122
H	-3.54652457251655	-2.86528431091957	2.68988516256878
H	-1.61452645144854	-5.95141577940905	3.40941797619006
H	0.75185498956664	2.67872738879094	4.72595051130231
C	0.40742759739937	1.67650253807695	4.98626157886993
C	1.52606162121871	0.73972881599827	2.97992951664702
C	0.17884360994814	0.84384212672605	3.72651991162851
H	1.88646582635179	1.72997632568296	2.69143473044752
H	1.17175448982594	1.22114361124941	5.61701401026757
H	1.43756566996345	0.14391344400515	2.07088677492073
C	-2.42787484845068	1.77526744622146	-0.42184641181698
C	-3.75879837383202	2.49505087129843	-0.65715979281548
C	-1.33980489645825	2.52438409336733	-1.23175258536997
H	-4.56165530810044	2.09310878023239	-0.03954201489736
H	-1.23732318289069	3.54849740343279	-0.86901313184924
H	-3.66895746787725	3.55396219333259	-0.41501344324846
H	-1.58295929272272	2.54884141111899	-2.29694850102861
H	-4.06502143381856	2.43386842705717	-1.70304331268612
H	-0.37548603933159	2.03064601565858	-1.11416903871988
H	1.42070723093520	-1.05303337315192	-2.11773751966882
H	0.11101429940547	-2.56140739837329	-3.65629425523468
H	-1.51405468208965	-5.02847667280200	4.89440444945305
H	-3.56533338010959	-4.62801428154685	2.67224051289848
H	2.27550930010702	0.26127986582326	3.61364407049826
H	-0.50691815143228	1.76701562218947	5.57271010865704
H	0.34601217421722	-0.79486533064492	6.18425226226653
C	-2.80099727462972	0.08814128510370	-2.32325853611460
H	-3.51803888294455	0.62886831858199	-2.92323652679904
C	-2.04748603304861	-0.99123300378449	-2.72865491807431
H	-2.09119735926185	-1.49918757838278	-3.67866769813765
N	-1.48072834188991	-0.53244394133349	-0.60111513797503
C	-0.82068493022924	1.52255225938729	2.83967171148312
C	-1.41205910982135	2.75278804188817	2.98781562251090
H	-1.29927022294035	3.42789687114417	3.82159144323079
C	-2.19148965205008	2.96539692173812	1.82929624343229
H	-2.76557415112091	3.85028242429671	1.59763959479107
C	-2.02689640240401	1.86049634012483	1.02751097119575
N	-1.19701370472880	0.95660769699892	1.65217675323723
C	-3.96230840828791	-0.77404364727985	0.32072441044758
Al	-1.37404050991572	-0.96566275944178	1.36675162623083
H	-4.60420227910545	0.11141829455872	0.36932633769924
O	-3.24012031419517	-1.03107331380225	1.33250560546957
C	-4.38903364599465	-1.80126971114972	-0.61928587656212
C	-5.21426520195011	-3.70293794482507	-2.49483355513055
C	-5.41763556826675	-1.51708779464128	-1.52614809469823
C	-3.79737958322605	-3.05701624794749	-0.66324120801058
C	-4.20155816353832	-4.00394098895578	-1.59782482150009
C	-5.83307230218701	-2.44568856065447	-2.44665371659807
H	-5.88214340129709	-0.53729857420270	-1.51062168882926
H	-3.03020795883236	-3.33048521254678	0.04503666797389
H	-3.69630774459650	-4.95986313792856	-1.59510918635398
H	-6.62901904220632	-2.22168084038350	-3.14506046490649
O	-5.67317034412672	-4.54862852059117	-3.44188451533562
C	-5.06468310521777	-5.80746436924551	-3.55105633240711
H	-3.99557231214422	-5.73321502708264	-3.77468462881810
H	-5.55742532758085	-6.32205122218882	-4.37396279834197
H	-5.18437937974323	-6.40704205358114	-2.64296450247687



[**1**$^-$]-*p*-methoxybenzaldehyde TS2 isomer A

N	-0.89868314737258	-2.58867839805871	0.78190188699013
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C	-0.54770867813271	-3.02391018872105	-0.47041189505583
C	-1.08604795448591	-4.82715924856766	0.72651308328328
H	-1.27059247483019	-5.84784086466207	1.02205960865751
C	-0.65191785312976	-4.39108675017857	-0.54294191679508
H	-0.43370071261273	-5.01196488766210	-1.39830211683545
N	-0.60834064505865	-1.39270490493727	3.22476241352381
C	0.06384731222244	-0.71894004292415	4.21111841706752
C	-0.93985898076573	-2.62586753583005	3.73105839738514
C	0.14741764096484	-1.50279890524262	5.33482709928758
C	-0.49794407185734	-2.72185122420018	5.02859162201256
H	-0.61389505771547	-3.56720131844262	5.68868274414007
C	-0.94796972487209	-0.88202545357770	-1.55404705133717
C	-1.99392792294033	0.87335169570988	-0.73043436603804
H	-1.04548873893921	-3.14141093936856	-3.16147007788988
C	-0.05487164750798	-2.76829444618240	-2.90029458330904
C	1.38667983359368	-1.63168221685228	-1.22565582006156
C	-0.05350605044174	-2.08379995994500	-1.53586380141917
H	2.04757368585137	-2.49926857371670	-1.20462914562563
H	0.63187508338933	-3.61473049585790	-2.90258745063783
H	1.45822821896978	-1.13978833866358	-0.25608935320703
H	-3.56600059408069	-3.39686224009571	4.03470031316674
C	-3.22105405667174	-3.36977398075161	2.99861440423687
C	-1.49573147150351	-5.03039875162714	3.58420602349085
C	-1.70524983845808	-3.65491169761877	2.94185294970099
H	-0.44465847142158	-5.31721864842374	3.57951622948398
H	-3.47477587656657	-2.39445431434703	2.59476598106327
H	-2.06603354132880	-5.79504881030174	3.05521895010926
H	1.49794529794120	2.26802351090192	5.11857463756298
C	1.02695708391818	1.29856230868958	5.28960380610567
C	2.03299797667038	0.40990173905292	3.20341283980510
C	0.70454902939392	0.61748747276668	3.96122737379881
H	2.51981772527602	1.36790055363233	3.00609190728135
H	1.72150731994102	0.69476179368757	5.87485245572602
H	1.87663583175892	-0.08301021520286	2.24332814317774
C	-1.75086832827716	2.22195908511063	-0.07698572533960
C	-2.94943846821919	3.15451527164234	-0.25765173794183
C	-0.55482465859144	2.84627222145846	-0.83808705573793
H	-3.81560702744023	2.83545868210219	0.31522620074302
H	-0.31240183094321	3.82194984491749	-0.41359743377625
H	-2.69313925525964	4.16396528716794	0.06465316339896
H	-0.78118123153310	2.97180966214690	-1.90035591239658
H	-3.24218147587699	3.22321736933041	-1.30700505949820
H	0.32854760544687	2.21500091173132	-0.74843587606977
H	1.75238177948512	-0.93063689647230	-1.98001732982313
H	0.27243378222750	-2.07728196776364	-3.67962115223752
H	-1.84860764980311	-5.02804684620758	4.61603035718814
H	-3.76937131222928	-4.12427970361874	2.42936004407392
H	2.70988876033598	-0.21673830506890	3.78760523429095
H	0.12674205353467	1.45239014400034	5.88467249432062
H	0.62608723735903	-1.24468772598171	6.26682934316661
C	-2.40657431275007	0.72515360655647	-2.07774926786588
H	-3.09206490483133	1.37617218571963	-2.60001751677454
C	-1.77474371813679	-0.38838107044386	-2.58849075118388
H	-1.89518779786039	-0.81837574799704	-3.57045824639378
N	-1.06298664355941	-0.13130494428045	-0.47055225272613
C	-0.19552081634422	1.49505400517415	3.14256571021952
C	-0.64504112934331	2.76547362639416	3.40670477294126
H	-0.46085969347408	3.34374571109640	4.29869586488550
C	-1.38924507426554	3.17209176241711	2.27559736354994
H	-1.86132096984378	4.13242280286448	2.13138910351520
C	-1.34533419827352	2.13576064963450	1.37305786437820
N	-0.62384931170171	1.09089399427542	1.90810807042283
C	-3.46724398394673	-0.31532256449669	0.31896458439580
Al	-1.05474329873600	-0.75697658855792	1.46654229517490
O	-2.90035516071580	-0.46838879608458	1.45119618672981
H	-3.31674950133737	-1.06634251679173	-0.46817915772209
C	-4.77004506878110	0.36641400308143	0.29628995510614
C	-7.26758891796328	1.61730404152707	0.25158393333592
C	-5.25504834901830	1.02241246185352	1.42955424721980
C	-5.55688838542012	0.34164506935921	-0.84595280395997
C	-6.79733949624059	0.95868328715584	-0.88223263161056
C	-6.48627108823196	1.64241096077470	1.40749535562977
H	-4.64705309748152	1.05266517324345	2.32400517053906
H	-5.18745306208257	-0.16271510843384	-1.73117591692556
H	-7.37783558516708	0.91548330741195	-1.79365192905995
H	-6.85959429327566	2.15566749835163	2.28418309023597
O	-8.45723105888968	2.25215404868152	0.32276719256827
C	-9.27959822529588	2.25788791815588	-0.81086881248064
H	-8.80648328752212	2.75085060636043	-1.66682667145445
H	-10.17506101887689	2.81593408018800	-0.54400718533630
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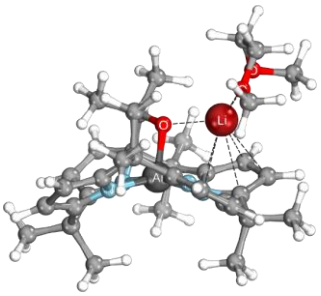

[**1**$^-$]-acetone Li(dme) isomer B

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C	-0.49598890036987	-3.05883696407447	-0.68341085783150
C	-0.85074901320151	-4.95787308877251	0.43918585176889
H	-0.90639553613861	-6.00306307434438	0.69738432689676
C	-0.40264466861864	-4.42419154857294	-0.78892804411665
H	-0.04041409874223	-4.98490524328673	-1.63642100370867
N	-1.07517112688420	-1.51958729844410	3.02248015203713
C	-0.41961665394545	-0.80379406438666	3.99631389403033
C	-1.14983932241257	-2.82364544873772	3.45823174220478
C	-0.09949941770938	-1.63583477801335	5.04127135237825
C	-0.56748953492566	-2.92450419817408	4.69775819332492
H	-0.47374542997559	-3.81784741585175	5.29412901661197
C	-1.16133540015884	-1.00721181505167	-1.75886373347432
C	-2.70648384496187	0.38864397054072	-0.91955903178536
H	-0.72212231799544	-3.17597541955323	-3.42863370604753
C	0.16708283660751	-2.66035943683770	-3.06515028676934
C	1.23492300066806	-1.32502188328681	-1.25089789695087
C	-0.06330430071170	-2.02469171668628	-1.69718633273770
H	2.03450517663943	-2.06235875382942	-1.18598901240715
H	0.97351588673440	-3.39005089350439	-3.00981788577991
H	1.13440736327454	-0.86230896107272	-0.26920204210004
H	-3.72478512921510	-3.83761662291007	3.58804135894508
C	-3.30893401145346	-3.76025583409019	2.58050438132255
C	-1.48149905168117	-5.27161124889103	3.27310624760104
C	-1.77509097687565	-3.91541498838938	2.62958989042508
H	-0.41122895914650	-5.46761939749686	3.32679452810626
H	-3.62192658200863	-2.80523702091094	2.16506669344993
H	-1.94864782856799	-6.07514815289586	2.70335038528537
H	0.32894679250674	2.37663938198647	5.07159416885973
C	0.01743870565425	1.33657508715082	5.17937299800962
C	1.38582016619106	0.70487105216288	3.19956807800438
C	-0.02454021372938	0.63781965513333	3.82066433300999
H	1.69503826925097	1.74015152532606	3.04119105481672
H	0.73497877643922	0.85159498469979	5.83997116893677
H	1.42092649467631	0.19417187106293	2.23735171225020
C	-2.26086379888543	1.83406109724033	-0.47517706640816
C	-3.28121571353329	2.91099978111633	-0.85515589906440
C	-0.95552757772233	2.21939510290217	-1.20478312761121
H	-4.22011607724534	2.84519086565001	-0.31533726385704
H	-0.66530849867789	3.21982082665694	-0.88392362566422
H	-2.86056433302387	3.89602821837433	-0.65232100684873
H	-1.07853595045895	2.24148371803580	-2.28899491112550
H	-3.50209320639853	2.88140996461999	-1.92264073452484
H	-0.12806482004306	1.55758959736010	-0.96047085036053
H	1.53683827629779	-0.54915425948022	-1.95861377459553
H	0.46103745257303	-1.90996578030508	-3.80137654731636
H	-1.89185846073786	-5.31422656013096	4.28266569399934
H	-3.74704582076724	-4.55104639381301	1.96834273771057
H	2.10860668013050	0.21997082319265	3.85668990609920
H	-0.95521913905946	1.31511810556052	5.67264278296681
H	0.42321358066238	-1.36386535238597	5.94502448696352
Al	-1.50582517706461	-0.98312187509772	1.23557701991310
C	-3.84652731229254	-0.34152158009128	-0.06645337576849
C	-4.22776302873291	-1.67006156503651	-0.73444553348023
H	-3.37925911091138	-2.33187247050879	-0.90559381730518
H	-4.74628195983340	-1.52273955509061	-1.68273117515467
H	-4.90677348034577	-2.19967418870145	-0.06510594639946
C	-5.12230694724291	0.48514300019820	0.04101144772509
H	-5.90955013555866	-0.13225052265117	0.47835027840131
H	-5.47805982446164	0.80599510063889	-0.93945978364623
O	-3.31648663945637	-0.60429473175658	1.20518616398738
C	-2.89371116594301	0.27552406449623	-2.39417654581758
H	-3.66258577660536	0.78294886936410	-2.95851591382296
C	-1.95812893050616	-0.54672366534211	-2.89049078834916
H	-1.82421709430523	-0.84763738845840	-3.91783671046462
N	-1.57294936471927	-0.46193220789907	-0.67505336217778
Li	-3.45186518498241	0.61896664396283	2.73886008354184
C	-0.97652181145699	1.35451952945954	2.90960387739535
C	-1.68869021530941	2.51521330952271	3.13044925304987
H	-1.70882260786713	3.09669829231709	4.03877548363784
C	-2.31628014501456	2.84106269626086	1.90096027636268
H	-2.91135004894776	3.71751952679883	1.69515859210632
C	-1.96113843091246	1.86329281035958	1.00065968970715
H	-5.00630087320976	1.36675004386892	0.66529925793422
N	-1.15385999449247	0.93524432473943	1.61937482427893
O	-5.20925216992295	1.81125540644834	3.12482465997618
O	-4.22975350055736	-0.30800104012611	4.41001299113812
C	-6.11237776540885	0.82661588075103	3.57243589452924
H	-6.28118698521889	0.16041709421489	2.72457754724082
H	-7.08058993656770	1.26423728454562	3.84810876058231
C	-5.54685656187841	0.04297239726569	4.73763395580036
H	-6.17068789749741	-0.84527213240738	4.90646668624278
H	-5.56813978483159	0.62806310673016	5.66825385562408
C	-5.11326544854228	2.93976442618272	3.96616330283037
H	-4.50592763448576	3.67957822722410	3.45228530967371
H	-4.63487159146215	2.71264369496824	4.92339264402540
H	-6.10256826673910	3.36815946929778	4.15886115717455
C	-3.62288768321299	-1.13272774250655	5.38815498822599
H	-2.58694250754800	-1.29316985268378	5.11103836355653
H	-4.13041458268235	-2.09951137560543	5.44978093489832
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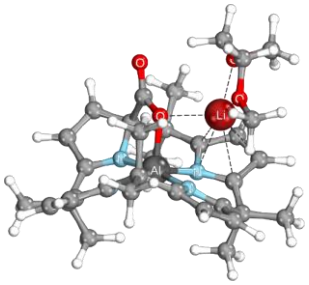

[**1**$^-$]-CO_2 Li(dme) isomer B

N	-1.00308269033928	-2.71525072595903	0.58955231160628
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C	-0.86433987068500	-4.95056697050553	0.47236389523486
H	-0.91592589372002	-5.99600146024002	0.72981966228861
C	-0.44774400119019	-4.41726955556572	-0.76721581088702
H	-0.10955208680140	-4.97854639687460	-1.62404211016832
N	-1.01108686592262	-1.53374681116126	3.07091240560089
C	-0.36025138497606	-0.83081727913495	4.05809173352687
C	-1.14185736864397	-2.83175004694002	3.51364148543606
C	-0.10280398106725	-1.66284724627604	5.11914175758066
C	-0.60481661847027	-2.93778996447490	4.77205854571676
H	-0.55760432628992	-3.82780016383603	5.37852334952638
C	-1.22707294311562	-0.98681932629185	-1.68742580545827
C	-2.67828336133013	0.45089755495284	-0.77458238248646
H	-0.90093724936163	-3.15534967328438	-3.38816689404919
C	0.01023016210005	-2.64857421680299	-3.07013440728914
C	1.18793243314920	-1.34176352555643	-1.30346147970788
C	-0.14166352003282	-2.01850637088565	-1.68867349967926
H	1.97758400188306	-2.09207378929269	-1.28367753807424
H	0.81178849819377	-3.38551195990023	-3.06067720499886
H	1.14600063380025	-0.88373542412449	-0.31524379139475
H	-3.71721709487952	-3.82681328513838	3.63286978457011
C	-3.30298909426968	-3.75740336542067	2.62415953974684
C	-1.47887884813006	-5.27583770484404	3.30773246986299
C	-1.76900702723859	-3.91427647695785	2.67310669041629
H	-0.40902560116667	-5.47297096224776	3.36523108430594
H	-3.62154588287879	-2.80840161604903	2.19985313717975
H	-1.94466541017903	-6.07446059043226	2.73033902799995
H	0.59783136210238	2.30346968836917	5.10130109473191
C	0.23269378704518	1.28262249187922	5.22139747820794
C	1.49524624978783	0.58050619693700	3.19770434844514
C	0.10519518301999	0.58681355443067	3.86704772289067
H	1.85258703574198	1.59830632559902	3.02847607975057
H	0.94644356135539	0.75876200473422	5.85574150442994
H	1.47552388809924	0.06927447336387	2.23479751104380
C	-2.27913787938094	1.90516466567992	-0.34048178322747
C	-3.44817889312301	2.86155018532607	-0.57841276612614
C	-1.08151960175081	2.37993476042476	-1.17712665241535
H	-4.32249392910161	2.61862365074620	0.02242336342729
H	-0.81692645823074	3.39146396442302	-0.86974184547094
H	-3.14683455713755	3.88150294872338	-0.34093744981472
H	-1.31167577220384	2.40419210651909	-2.24373432847912
H	-3.74578913073023	2.86161948121566	-1.62708875845533
H	-0.20150192664688	1.75735848713885	-1.02497386448353
H	1.46647902997373	-0.56597063261610	-2.02061424701014
H	0.27211698060802	-1.89709324336223	-3.81723550588196
H	-1.89426740385405	-5.32675368611185	4.31464727419319
H	-3.74251548891203	-4.55237338891234	2.01925154974187
H	2.21301812710534	0.05775003872877	3.83057344554495
H	-0.72093420816239	1.31561859533623	5.74975648579527
H	0.40456331618183	-1.40210792899946	6.03473910575782
Al	-1.41835506588996	-0.98208580490254	1.29816277092221
O	-3.27675810077438	-0.62659726910498	1.26015462860327
C	-3.00746625776942	0.28303933426682	-2.21687831443442
H	-3.83782597716353	0.76178740054632	-2.71205506918915
C	-2.11702759679979	-0.55690235850372	-2.76083859940425
H	-2.07716248018591	-0.90068389282529	-3.78221637092290
N	-1.53880207724688	-0.40397151153220	-0.58702686820826
Li	-3.26422796981826	0.78108488968328	2.84557227944165
C	-0.83782721624910	1.35501263356843	2.98860812861864
C	-1.45056975148136	2.56914040947777	3.22125047971960
H	-1.39402398207473	3.15890890209989	4.12212893172254
C	-2.11073387498519	2.92377223935652	2.02130476536246
H	-2.65694343800219	3.83566434317707	1.83887223110387
C	-1.87814352270966	1.91197430539993	1.11630352923735
N	-1.11318700584164	0.93177904964032	1.71591727597050
O	-5.09105135776294	1.69439857624496	2.78977500312618
O	-4.12663576942699	-0.19981800655661	4.35287765348357
C	-5.95555810121702	0.62197914117343	3.11249187873848
H	-5.90019816538954	-0.07363857268616	2.27587902438119
H	-6.99508339664874	0.96258674852853	3.19392425568934
C	-5.52436987822089	-0.05218741374162	4.40122835409522
H	-6.02517980848398	-1.02562209424446	4.47936000380758
H	-5.81226850129440	0.53010599404996	5.28797145776594
C	-5.31160108186879	2.86871308299792	3.53753367337771
H	-4.64149344474196	3.63271800111221	3.15124515886317
H	-5.10164891762976	2.73856922635836	4.60409257072190
H	-6.34327403131513	3.21616808018911	3.42355828349089
C	-3.60176380773765	-0.96746903587745	5.41896031999341
H	-2.51849763358754	-0.97720994981819	5.33141398141456
H	-3.96447093233269	-1.99752762276391	5.37370562851619
H	-3.88249546595280	-0.53322452728551	6.38479884164354
C	-3.77358918585620	-0.08772537151830	0.17795433983434
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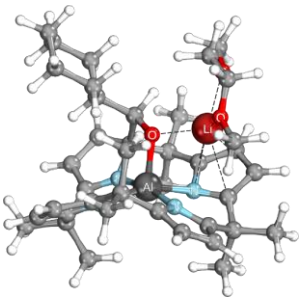

[**1**$^-$]-cyclohexanecarboxaldehyde Li(dme) isomer B

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C	0.43302907551474	-2.60133671901676	-0.95170818368431
C	0.20442360063610	-4.62327100752698	-0.03238570332870
H	0.23138980136491	-5.68997646585416	0.12138456143575
C	0.61602854867093	-3.93956651807878	-1.19676026334034
H	1.02271240884715	-4.38567865336659	-2.09089024053662
N	-0.35555558581426	-1.44162259904007	2.85042135501329
C	0.16693690147969	-0.71819424532205	3.89820780986155
C	-0.21585771976184	-2.77347878700925	3.17729343562379
C	0.61759890034997	-1.57300584756535	4.87282595136926
C	0.37016540964122	-2.88506442814118	4.41295156039248
H	0.60410229491601	-3.79915783641396	4.93442078340320
C	-0.34390087553782	-0.50838788335760	-1.86065033491787
C	-2.08641722786825	0.61775699884148	-1.00400227311458
H	0.36599335599259	-2.44655722931424	-3.70607835664258
C	1.18886548556761	-1.90759239822780	-3.23566350572976
C	2.03939738091710	-0.68978687919895	-1.23378223511729
C	0.83063944373538	-1.43702583978337	-1.82906346584847
H	2.89169012777591	-1.36693028369423	-1.18687581219081
H	2.04625125677727	-2.57791463300067	-3.19940559926101
H	1.84590016169164	-0.33694415816210	-0.22092055067153
H	-2.54471970512142	-4.22847562059188	3.36959899566737
C	-2.23870822180233	-3.96355411748166	2.35478012899958
C	-0.16293253634882	-5.22181306463018	2.79339046353619
C	-0.70136426043518	-3.88231508123180	2.28314815362815
H	0.92574247167867	-5.24997327165413	2.77485737806885
H	-2.71653381915877	-3.01882616095782	2.10677422453245
H	-0.53745659038185	-6.04332719142423	2.18240400173231
H	0.25807174338833	2.41753278379413	5.30658713122208
C	0.16240883369815	1.33066621188322	5.30354094217887
C	1.65781220293182	1.18759553295751	3.32136683224033
C	0.28016148324576	0.78046061291379	3.88225889468300
H	1.75927088417901	2.27421062275969	3.28103405128880
H	0.95451037357593	0.93433296777397	5.93754583290602
H	1.80849706227343	0.80002566071683	2.31403604478134
C	-1.94874488150389	2.03867483617418	-0.36752080641731
C	-3.17224178296924	2.88722918263817	-0.71249611525520
C	-0.71023776475926	2.75933918791356	-0.92721147329974
H	-4.11037365992125	2.43360023734887	-0.39519161106192
H	-0.62930988933710	3.74061413661301	-0.45919911861834
H	-3.09930657422937	3.86477988856013	-0.23676314927489
H	-0.77316522241400	2.90795355072570	-2.00674415667790
H	-3.23578196538916	3.06748562589865	-1.78588873053657
H	0.20920485754539	2.22156789721713	-0.70390190670166
H	2.31692127920859	0.17362596347321	-1.84321514686910
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H	-2.61660357491968	-4.72887906967645	1.67343335231901
H	2.45150987432487	0.78581428522298	3.95225202958809
H	-0.79197084902661	1.06678445904112	5.76087866656709
H	1.08129011214432	-1.29704302317202	5.80703862879981
Al	-0.83650105826645	-0.82716675383669	1.09497586264195
C	-3.18683719583347	-0.27661883439668	-0.28113555438134
O	-2.66816232130849	-0.73543581908591	0.93065950702663
C	-2.14098008127291	0.67839149312162	-2.49417019762387
H	-2.88797981963541	1.20602780474789	-3.06662444470760
C	-1.09273597179254	0.01306348511105	-2.99753927161038
H	-0.84351223670552	-0.13257472270803	-4.03691341515662
N	-0.87773277996746	-0.12368254731515	-0.76016448508114
Li	-3.12910652670552	0.33111216364379	2.52274572506517
C	-0.78172494239281	1.38333499861832	3.01467713619212
C	-1.73473337624022	2.32937084798786	3.32672146097817
H	-1.92124172437798	2.76820532881808	4.29383681101737
C	-2.36875516659011	2.67594724924548	2.10591559527319
H	-3.12223696023357	3.43762982149785	1.97590141516056
C	-1.76943933115428	1.92173090138084	1.12059867384685
N	-0.82056013365952	1.09623102509263	1.67801602854973
O	-5.17674904607609	0.72935477299399	2.56487336546283
O	-3.70517619091123	-0.93338043309446	3.99055858307201
C	-5.75097749931143	-0.51975996348882	2.88217621148622
H	-5.60383963528623	-1.22833997517846	2.05718818146816
H	-6.83067921448814	-0.42700299357734	3.05645396330726
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H	-5.41367878672508	-2.05194658460988	4.32976212395484
H	-5.42256971876380	-0.41392450855918	5.00469710418332
C	-5.94953668873119	1.50122509834663	1.67984895383014
H	-5.41107577884996	2.42794307172791	1.49556255562933
H	-6.92519151758798	1.74247339604143	2.11466653338232
H	-6.11394178889534	0.99209698962749	0.72344269680297
C	-2.99672396280263	-1.45921971869999	5.09749007733835
H	-1.93340771711586	-1.32965303406464	4.92080170101320
H	-3.20351853099528	-2.52622970467561	5.21772831594190
H	-3.27491978392233	-0.93767515153540	6.01989922129166
H	-4.04179455332369	0.38278996415628	-0.07241426209058
C	-3.70680123054738	-1.40180565471898	-1.20391298823766
C	-4.65665693657330	-3.72595904689158	-1.40923940569018
C	-5.39349792640794	-1.94899468941579	-3.01897826615993
C	-5.79877455244445	-3.21796270342140	-2.27954491197223
C	-4.87968415223647	-0.89309460947844	-2.04772129648317

C	-4.13780599875098	-2.65725883662009	-0.45199945171207
H	-3.83089905680925	-4.05757939303812	-2.04771783762785
H	-4.60766583059379	-2.18360584021866	-3.74495221157763
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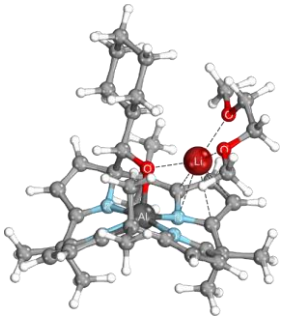
H	-4.91624862337549	-2.41261137996462	0.28191996571546
H	-2.90440563598460	-1.71941111639285	-1.88145779505379
H	-4.97242862355560	-4.60503800520828	-0.84249546880128
H	-6.23565358370490	-1.55409047200738	-3.59263637881387
H	-6.11356999769829	-3.98795825093373	-2.98791365112192
H	-4.61762472687402	0.01412060204415	-2.59737818748429
H	-3.29610716849582	-3.05815342014066	0.10508231063329



[**1**$^-$]-cyclohexanecarboxaldehyde Li(dme) isomer A

N	-0.13269210150766	-2.33801273922233	0.06243020388047
C	-0.15561136349548	-3.61234188133606	0.56778188088884
C	0.52274480984475	-2.40002202387544	-1.14426357405015
C	0.47023374343255	-4.46901964813934	-0.30549133161045
H	0.60330071841335	-5.53189408769284	-0.18411354113950
C	0.90440980116857	-3.69268067772083	-1.40190878484845
H	1.44326147012183	-4.04909308068982	-2.26585052410831
N	-0.56571191425761	-1.56127287792758	2.65394207810057
C	-0.17506880542552	-0.91812241750412	3.80189658618746
C	-0.52498915870147	-2.91382712333565	2.90791625903698
C	0.08885460994193	-1.84457922560461	4.78028442679985
C	-0.13913204209096	-3.11780378915251	4.21091474178291
H	-0.01172818306791	-4.06899130598848	4.70259990189559
C	-0.42749095229251	-0.34934953516599	-1.98547000608166
C	-2.22111774189666	0.68898744553568	-1.10470809431226
H	0.48143270275523	-2.15504978891455	-3.88708458764376
C	1.24160486948231	-1.55441337244720	-3.38721520506083
C	1.95139507998561	-0.33920680115647	-1.33014457573424
C	0.82353069046185	-1.17224121703966	-1.97010171834138
H	2.86141071997864	-0.93736009667093	-1.29528471891237
H	2.16048170353761	-2.13813303330976	-3.36269077701920
H	1.71357763764566	-0.04273452301468	-0.30860517894362
H	-2.89466126614398	-4.32184999210021	2.53853523324629
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C	-0.85953542005157	-3.94412381152677	1.85872905576744
H	0.66863952099513	-5.35237461686968	2.51832400916211
H	-2.80901580094678	-3.08271714418566	1.28722974290127
H	-0.65650224162563	-6.08818826819603	1.60902849349926
H	0.12190926837690	2.14536166039025	5.33717560964229
C	-0.07050301641819	1.07299735834136	5.28307141099009
C	1.49866060115273	0.86322123011849	3.36490887988944
C	0.06395972452868	0.56735912300228	3.84782371127068
H	1.70116948266637	1.93631049277652	3.37298515028023
H	0.65222557419806	0.58159564447019	5.93330045192065
H	1.66104542176533	0.50000389278605	2.35008695670228
C	-2.05777407265605	2.08955024941129	-0.42123888148643
C	-3.25726653874780	2.99100130243983	-0.71279846333250
C	-0.82075268125400	2.80971351344359	-0.99496574603748
H	-4.19510447221786	2.60003831597045	-0.32598116336752
H	-0.73714354602635	3.78780844074060	-0.52075017315695
H	-3.10040463903386	3.97590278080533	-0.27294196071456
H	-0.89530051812256	2.96733180251922	-2.07259113171447
H	-3.37609695987880	3.14667952749525	-1.78573073542282
H	0.10285686575150	2.27483694268703	-0.78436338966445
H	2.15628689084644	0.56833970341220	-1.90343294360618
H	1.44031114816429	-0.66707408868706	-3.99124925635473
H	-0.91427850233560	-5.58964468393645	3.27030259948392
H	-2.59960196661478	-4.77552884908476	0.85515194881922
H	2.22202938365488	0.36524228964122	4.01144165929046
H	-1.06616104429135	0.87954453989924	5.68507917525785
H	0.42935915250043	-1.64646642900620	5.78431634974646
Al	-0.95183492984859	-0.81738085451812	0.94055768901960
C	-3.24457412785335	-0.35760213130632	-0.47482211221005
O	-2.78627380542688	-0.69950951662690	0.79666123151496
C	-2.28447226532358	0.75748491516024	-2.59647104258896
H	-3.05998863661683	1.24386950120974	-3.16634999183926
C	-1.21540120164220	0.13455576556987	-3.11072640836059
H	-0.97412001099192	-0.00221276921166	-4.15324809774725
N	-0.98086668983677	-0.01670084671577	-0.87864806981655
Li	-3.30895586739532	0.42849849420660	2.36006781037205
C	-0.89763127272353	1.30192040503405	2.95940722604210
C	-1.76524752695775	2.32494945468835	3.27781070123066
H	-1.92732042031772	2.75961249593593	4.25111746314165
C	-2.35942209770629	2.73922124656394	2.06107730871033
H	-3.04724808139859	3.56161653178561	1.94184607999853
C	-1.83477968429738	1.94476198122279	1.06476661377372
N	-0.94248504062505	1.05018223952253	1.61623299491074
O	-5.16340509852822	1.51431623541852	2.88104690801772
O	-4.08286535894661	-0.72033030036188	3.84521296911012
C	-5.91245118442672	0.76816719453917	3.80847867062688
H	-6.59601337744205	0.08221584794689	3.29012438256719
H	-6.52075541467402	1.42531106149718	4.44443892670077
C	-4.95080738736828	0.00288548440916	4.67793302270564
H	-5.52527740690735	-0.67020560128113	5.32784837623246

H	-4.38585549642723	0.68656300537493	5.32618057570252
C	-5.93027702445341	2.47671030860398	2.20223669929638
H	-5.26879149176715	3.01995320085608	1.53221949832078
H	-6.37950622131021	3.19138133755314	2.90042481970583
H	-6.73161708824689	2.01967879686727	1.61074769319527
C	-3.36032920855926	-1.72216497712408	4.54478558915481
H	-2.72300502094748	-2.23917173137913	3.83631591709333
H	-4.05191340864588	-2.43962471830496	4.99802081456459
H	-2.72573688208350	-1.28971296093536	5.32122671188172
H	-3.15194640505846	-1.22376841102859	-1.15443755648007
C	-4.74139417590995	-0.03016358127162	-0.42328070533704
C	-6.85152563514774	0.57121639734535	-1.69887764489060
C	-6.99421529467766	-1.03320608940753	0.21192853350133
C	-7.57320921227638	-0.64694287095485	-1.14141906179455
C	-5.48755484094573	-1.24914412702426	0.13958196148795
C	-5.34241193174298	0.35623030778758	-1.77451376139425
H	-7.05716789757150	1.43770285450602	-1.05909820490172
H	-7.21569723582306	-0.24101202719481	0.93744553472088
H	-7.46091088032364	-1.48601783149083	-1.83610032331796
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H	-7.47773236909684	-1.93616903094702	0.59198441647407
H	-8.64543451610102	-0.45248588808316	-1.06247156957426
H	-5.10315658710587	-1.50855036427255	1.12571049095268
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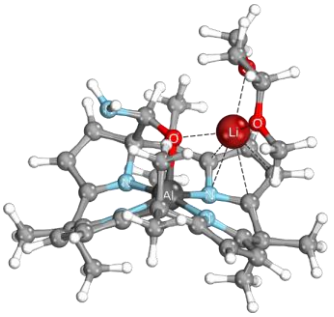

[**1**$^-$]-formamide Li(dme) isomer B

N	-0.23321846591480	-2.27990643849878	0.12124546544553
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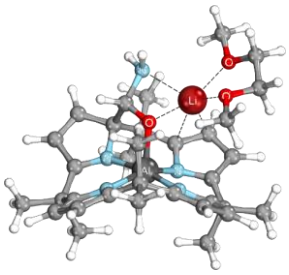
C	0.08370017585107	-4.46131814591699	-0.29877560947761
H	0.10412902550211	-5.53380769942665	-0.19067073969113
C	0.52635858533476	-3.72678222243378	-1.42051774379909
H	0.95605756524738	-4.13283287385050	-2.32283893425659
N	-0.49173101062270	-1.45670397466820	2.72688533766473
C	0.07032482074000	-0.84378948575686	3.82132829795864
C	-0.48476428280357	-2.81099426307378	2.97499304466890
C	0.41547953441103	-1.79064501810660	4.75432614720369
C	0.05718068871828	-3.04626819765450	4.21420217202986
H	0.19744954064884	-4.00672622835596	4.68362219667570
C	-0.46372850569235	-0.25998718106595	-1.92222947239162
C	-2.11196498345677	0.90446244393031	-0.95859429608727
H	0.15067035071756	-2.13922201614190	-3.86578126874732
C	0.99549466287460	-1.62285195811843	-3.40974157651409
C	1.93548122922822	-0.49556438665414	-1.39473229073097
C	0.69592795056178	-1.20627826176703	-1.97249981383820
H	2.78175979695465	-1.18160753750707	-1.41261150620605
H	1.84961865665320	-2.29784051585136	-3.43512435779382
H	1.78486385382789	-0.18665695853629	-0.36048738204242
H	-2.96921549140611	-4.03236724426918	2.84886987934472
C	-2.52986436904351	-3.77460441574598	1.88194903512927
C	-0.60852023667038	-5.22440357498726	2.43075284053251
C	-0.99014332182633	-3.81559215131727	1.97301222060167
H	0.47185864328894	-5.34361109134722	2.50255517262118
H	-2.90506922827476	-2.79334113678226	1.60140128136368
H	-0.98959634254632	-5.97056029277163	1.73318628295448
H	0.48713540619356	2.19515705667408	5.37856184657534
C	0.28951264139127	1.12350933743508	5.32524262163206
C	1.72627574586169	0.93918983572074	3.30440226363195
C	0.32675773003910	0.63738406364607	3.87690861934401
H	1.93056496521563	2.01190898535433	3.31328221564579
H	1.05351656328528	0.62288705492135	5.91883841201952
H	1.82262174755151	0.58962846723064	2.27654088727837
C	-1.93137703085812	2.27715620112054	-0.24618238878622
C	-3.15276603135221	3.16223842071016	-0.49241343706769
C	-0.70497157652179	3.00569760939647	-0.82207075760418
H	-4.07979582683314	2.71741009927383	-0.13421159398294
H	-0.59288336878651	3.96729355069021	-0.32055885882970
H	-3.03227934380048	4.12212508020572	0.00909068825862
H	-0.80672572290444	3.19468293257395	-1.89251884814792
H	-3.27222032494263	3.37820385544451	-1.55459597365206
H	0.21337969784394	2.44611018601650	-0.65507028201274
H	2.19783110579578	0.39222792614941	-1.97537366661324
H	1.25077421478611	-0.75747737514595	-4.02433191218605
H	-1.04590406495126	-5.44339163173658	3.40558889331420
H	-2.88090247092417	-4.49777834299940	1.14280025359966
H	2.48931656925366	0.43304273162348	3.89675032381526
H	-0.67590450394845	0.92739090954497	5.79338247017554
H	0.88041125023849	-1.61291392067662	5.71154482059340
Al	-0.89566624132886	-0.70210793513938	1.01287440968517
C	-3.20723360462116	-0.02993522544524	-0.28869643809123
O	-2.73703661906336	-0.48634963111800	0.92551237293462
C	-2.24824186033672	1.00180054704860	-2.43807533744461
H	-3.02746170591807	1.54432125555524	-2.95395654485375
C	-1.25778500530953	0.30408959143534	-3.00749986908617
H	-1.07988650467395	0.15144832568346	-4.06042605033183
N	-0.91861307870088	0.12595115584333	-0.78754831883153
Li	-3.08758835479678	0.51639235284371	2.58430774007724
C	-0.69275057949411	1.37879251910438	3.06487156175658
C	-1.57468870237814	2.36536448536875	3.45297540367863

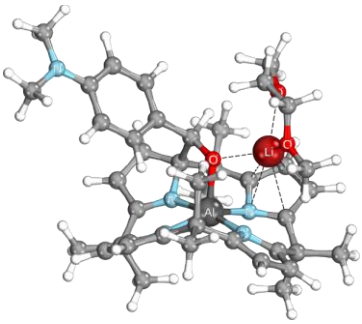
H	-1.71032848800339	2.76021415300399	4.44718640614878
C	-2.21598461198686	2.81599545116008	2.27027457804655
H	-2.92320744116676	3.62853423846710	2.20282523833709
C	-1.69266256172379	2.08028695623671	1.22849784422789
N	-0.78032830249616	1.17277386563434	1.71619630394047
O	-5.13967752794735	0.99094065775813	2.64892335293254
O	-3.75665372713588	-0.84703582792955	3.91413819717995
C	-5.73188937574657	-0.28587673107590	2.74512155954641
H	-5.53690760169554	-0.86772571123704	1.83516889429654
H	-6.81990774251177	-0.21076469441324	2.86858572050052
C	-5.15124438510003	-0.96547637868934	3.96117845426883
H	-5.46242261856765	-2.01864392540615	3.96670657012521
H	-5.54498591688167	-0.49993095193394	4.87551539012343
C	-5.87125581305627	1.90490083759519	1.87249959211779
H	-5.32424515013078	2.84471717303787	1.86846787083742
H	-6.86539304445092	2.07901363730791	2.29747803303127
H	-5.99349183654552	1.56423104133038	0.83810115784166
C	-3.11296989421567	-1.49738216852486	4.99343916968089
H	-2.04452979082038	-1.31862203808300	4.91452456919074
H	-3.28616270432002	-2.57619417525470	4.95681915868739
H	-3.47631527828308	-1.10968190877128	5.95167253816732
H	-4.11391370705684	0.58151447064711	-0.13241680683148
N	-3.44173908948082	-1.15819597477824	-1.15459830703757
H	-3.74750562024952	-1.95213182277232	-0.61077555078920
H	-4.11972416021376	-0.96929036840728	-1.87890540325958



[**1**$^-$]-formamide Li(dme) isomer A

N	0.01207833743043	-2.31540700271501	0.05647135268136
C	0.05803850389166	-3.59712113636993	0.54399704996224
C	0.67208579286822	-2.32440599101233	-1.14993353271141
C	0.73868157359943	-4.40309956154453	-0.33745906279415
H	0.93076045169795	-5.45856681535763	-0.23204261055369
C	1.13057472207777	-3.58926912569640	-1.42143289636968
H	1.69052749123258	-3.90400825973301	-2.28814878586246
N	-0.47400672755792	-1.63873266671659	2.66405636001573
C	-0.18937709677932	-1.01129908178046	3.84917413771784
C	-0.45880197320370	-2.99277650818766	2.89856900988367
C	-0.02824062187721	-1.95140449915275	4.83746518301660
C	-0.20662375985002	-3.21655675874445	4.23093250888045
H	-0.12397338605606	-4.17404747634456	4.72000254694063
C	-0.38323702856605	-0.30639028643971	-1.96117723058378
C	-2.18024592359517	0.66976834332504	-1.03729594648603
H	0.56732840188641	-2.06177791410121	-3.89138515342721
C	1.30819187143911	-1.43003656132278	-3.40087726922407
C	1.99981523119424	-0.19689782496161	-1.34702601789447
C	0.89993588715539	-1.07770606450071	-1.97295643895783
H	2.93789207846860	-0.75102201339301	-1.33972250329046
H	2.25346062247416	-1.97030036325810	-3.39938932564491
H	1.76912086007254	0.07345528578022	-0.31671332771002
H	-2.69766312708101	-4.54716144542497	2.37646268701908
C	-2.16444142474742	-4.20317234634907	1.48685577625784
C	-0.13102560613211	-5.36407494766778	2.27237825979538
C	-0.66607613801055	-4.00947732258625	1.80243281204092
H	0.93391499822857	-5.31751388608555	2.49649489684124
H	-2.63905559968658	-3.28661274875960	1.14066252724650
H	-0.29123130772465	-6.12729826360798	1.51055139963676
H	0.12422241038832	2.02857218871513	5.42629847621578
C	-0.06849154989346	0.95702801050559	5.35951680990552
C	1.50849862513968	0.75473048042251	3.45069101651799
C	0.06637237085330	0.47031412442145	3.91816513546436
H	1.72325785743552	1.82510419422429	3.47807088196761
H	0.65426472106947	0.45597445734437	6.00276812957997
H	1.67657060646882	0.40672693692448	2.43145210870752
C	-2.04459934990511	2.05942855447271	-0.32586323961355
C	-3.25057880732101	2.95847017073958	-0.60562638289101
C	-0.81025384370227	2.80099608680788	-0.87560109245964
H	-4.16893093199647	2.58581901030555	-0.16029006701058
H	-0.74496202429797	3.77135596578536	-0.38350902726033
H	-3.07057529870652	3.95245889423546	-0.19685898614924
H	-0.87462542947559	2.97586010098551	-1.95158225900849
H	-3.40845768186729	3.08827043072573	-1.67762034838319
H	0.11731584142520	2.27521761000166	-0.66138861453452
H	2.14863384026126	0.72655555192973	-1.91230800711332
H	1.45484989381428	-0.52977803208431	-4.00091466546442
H	-0.65701543660862	-5.69441171776056	3.16844762341229
H	-2.28769196852430	-4.95447541285231	0.70447346259376
H	2.22087569527563	0.23759931253445	4.09465551915579
H	-1.06378129676974	0.75983741715739	5.76039417415739
H	0.22168380705949	-1.76652034644704	5.87056089278727
Al	-0.87122432810393	-0.85504266964433	0.98082385786457
C	-3.17874098777172	-0.38930408199809	-0.42121493246501
O	-2.70598613006278	-0.86112076860416	0.77996255747636
C	-2.28624912145956	0.75679592691004	-2.52451631126656
H	-3.10001578080516	1.21869353252401	-3.06503269127981
C	-1.20756851033262	0.17668012221377	-3.06775314851563
H	-0.98130903339405	0.06026359347631	-4.11624205946063
N	-0.93150430581873	-0.01593603893421	-0.84143366347063
Li	-3.75805758267426	0.40777014900136	1.94249184560316
C	-0.88673145071319	1.22167188082927	3.03346752401022
C	-1.77723662793074	2.21658306276541	3.37020717074022
H	-1.94509414102540	2.63165577020933	4.35135732575877
C	-2.39296700681404	2.63054510779703	2.16514702295358
H	-3.10467990249732	3.43443636641432	2.05695980281451
C	-1.84527808884598	1.86957257413348	1.15558458772730
N	-0.92483886843002	0.98968954994124	1.68759468779925

O	-5.36322952972149	1.57804004889466	2.73820839033163
O	-4.29915181954483	-0.68936713162310	3.54208948022438
C	-5.86818794060646	1.01683441393609	3.92376542521734
H	-6.74826935910255	0.39444113338037	3.70856006834213
H	-6.17877300069342	1.79658352938180	4.63198804219851
C	-4.77622920566735	0.17845414922187	4.53904561803335
H	-5.19481752004374	-0.38093827913177	5.38588351770277
H	-3.96327574640169	0.80819475430323	4.92335522965075
C	-6.29086916023430	2.38220193846349	2.06084455373665
H	-5.80202844636068	2.78472448133267	1.17689462781942
H	-6.62648970155572	3.21955191892775	2.68233144714084
H	-7.17254496293218	1.81199162571649	1.74566101703319
C	-3.53815119285181	-1.77256672896503	4.05918561701210
H	-3.20407184781597	-2.37108943455892	3.21970989217870
H	-4.15913712757870	-2.38936942018255	4.71680497508573
H	-2.65711003790387	-1.42867766234197	4.60539071705505
H	-3.21664172267617	-1.20233552093255	-1.16705060356303
N	-4.50468843972717	0.15642382663337	-0.16274033872964
H	-4.85372346180668	0.70393713816337	-0.93866446695647
H	-5.15104506306669	-0.61548332843314	-0.04003473280662



[**1**$^-$]-*p*-dimethylaminobenzaldehyde Li(dme) isomer B

N	0.21810892003407	-2.42758044505261	0.67638247902824
C	0.14945103699275	-3.62102707496100	1.35068866521368
C	0.79760075054301	-2.68848758376456	-0.54263534214481
C	0.66671066810599	-4.62424587492060	0.56492557331761
H	0.75175446254773	-5.66749835817002	0.82318409914656
C	1.08177807512161	-4.02725517937264	-0.64571060959625
H	1.54955387135647	-4.52750991069598	-1.47918423152075
N	-0.26279808746788	-1.25380959883323	3.10823912863541
C	0.17389229052031	-0.42282456003711	4.11151813459506
C	-0.11458851953549	-2.54559095485882	3.56093777984004
C	0.58180214906566	-1.17202470415050	5.18770976446423
C	0.39458962603558	-2.52753873487160	4.83585345137261
H	0.61951350566143	-3.38356800852877	5.45159520567974
C	-0.16927185041863	-0.80021855101100	-1.68479509309167
C	-1.96800491897234	0.31547647029379	-0.95165998797081
H	0.72523555850611	-2.86502412800940	-3.29246370509766
C	1.49407013674741	-2.20117513743862	-2.89646071169595
C	2.21676277944611	-0.67767733195922	-1.05893197345298
C	1.08867483073773	-1.60362398500836	-1.55244004921207
H	3.13217075896747	-1.25765389502981	-0.94468160051919
H	2.41113283754713	-2.77891433656557	-2.79037862774495
H	1.98736924398831	-0.23200387850232	-0.09119720758219
H	-2.44055226045353	-4.03883344571629	3.59732514295314
C	-2.00595587621608	-3.89131812003130	2.60552683457088
C	0.04889875976118	-5.01147182725342	3.39604733733677
C	-0.47449076259745	-3.74208359319896	2.72061522644861
H	1.13342716738973	-4.99488720579722	3.49705752415850
H	-2.48253045013942	-3.02198474344348	2.15915753647096
H	-0.22845540198908	-5.89492431533858	2.82068607231087
H	0.12903606254178	2.84141619780040	5.19373926342742
C	0.06133196793159	1.75745516101812	5.29764073287183
C	1.64616396753750	1.45413527513073	3.40541631426970
C	0.25469669033563	1.06976102758001	3.94630911624269
H	1.72492328225342	2.53321859028013	3.25735024109171
H	0.83511142401275	1.44963652089255	5.99994775755092
H	1.85207957567896	0.97006469022576	2.45099112694846
C	-1.88282737835898	1.80700848293061	-0.48807873185710
C	-3.13026550018726	2.56813936364300	-0.93612654691185
C	-0.66489475037577	2.49942834728908	-1.12113900475725
H	-4.05630293069270	2.13346716639102	-0.56031402072852
H	-0.63713250351980	3.53850475641998	-0.79212148318008
H	-3.08755460153787	3.59976524446136	-0.58779365151310
H	-0.71208723591709	2.49439823725421	-2.21164494873093
H	-3.19518328476058	2.60544817378696	-2.02390718717959
H	0.27226449019407	2.04108353401853	-0.81190139949018
H	2.40780421877268	0.13328395255195	-1.76567487354106
H	1.68923583598725	-1.41703688812367	-3.63022623791248
H	-0.38932071895132	-5.12697974640927	4.38803875245955
H	-2.25604037997468	-4.75867668347168	1.99116270231120
H	2.41935199897320	1.14057697323665	4.10770356355238
H	-0.90459171937209	1.51315289572638	5.74148354289183
H	0.97927839979016	-0.79923796905936	6.11889391848730
Al	-0.66660674848557	-0.81276713201878	1.28919139990354
C	-3.03452358423615	-0.51138226976569	-0.12663592442617
O	-2.50042361891862	-0.84244713215510	1.11574279232232
C	-2.05837830780035	0.15681924501125	-2.43146007615172
H	-2.87745033882394	0.50759720951067	-3.04081893245156
C	-0.96967748896568	-0.49239211999093	-2.86408434242154
H	-0.73524293878513	-0.78139400079903	-3.87623327778937
N	-0.72429650223667	-0.32558670788995	-0.63081429412647
Li	-3.06662209034401	0.31426849297785	2.59676544607137
C	-0.78574576554433	1.54851827108885	2.97820835377505
C	-1.80809838031091	2.45356831925206	3.17066357381207
H	-2.05964023352453	2.96285966416205	4.08737113542177
C	-2.41048901267436	2.65289449574693	1.90117873638296
H	-3.20252352546918	3.35097298289286	1.67690869581357
C	-1.72416329225089	1.86011134022413	1.00772999591408

N	-0.74760028952547	1.15081063277174	1.66959797906837
O	-5.14694162138950	0.50548643738501	2.47201773912588
O	-3.62848164406790	-0.90356556574501	4.07781036543613
C	-5.55856527725626	-0.82586696436443	2.71205114191716
H	-5.21018026934486	-1.48405761631962	1.90662223747322
H	-6.65247159705399	-0.89935906809884	2.75774157058450
C	-4.98884035543356	-1.24111801815251	4.04743573997147
H	-5.13304038930768	-2.32160955359442	4.17785783734925
H	-5.52495168412191	-0.73393880222284	4.86181166307648
C	-5.94630785317147	1.19381953181302	1.54406649883432
H	-5.51086696999427	2.18072327837903	1.40186842518208
H	-6.97013435670585	1.31196723307533	1.91442059751677
H	-5.98906503929025	0.68366227809520	0.57512578411343
C	-2.98386640919425	-1.30611898343268	5.27004340025993
H	-1.94692888649892	-0.98513845798460	5.22395166961905
H	-3.00340848855367	-2.39392762641737	5.37589882261154
H	-3.46625164222781	-0.85378581563162	6.14387408257540
H	-3.89873884014913	0.15447258344987	0.00238953839612
C	-3.52212766969497	-1.71142115606538	-0.89976004632628
C	-4.43415626618302	-3.87936779346084	-2.49225519805763
C	-2.83548567977244	-2.92008990390781	-0.93167139807301
C	-4.67605777439698	-1.61618170790620	-1.66641383622863
C	-5.13089592730008	-2.66170128944654	-2.45089236925222
C	-3.27167073820906	-3.97544669888879	-1.71023545704280
H	-1.93802616390370	-3.06452920672903	-0.34635607311287
H	-5.24638432996422	-0.69150578440854	-1.66290991701567
H	-6.03718131563520	-2.52074899752136	-3.02259516379264
H	-2.68388854796715	-4.88213912640439	-1.69611124512067
N	-4.87522247453884	-4.93409630090177	-3.25540581180522
C	-4.05862846791127	-6.11290916720253	-3.37495581136988
H	-3.07998557738929	-5.91330315100886	-3.82643471141185
H	-4.56802768347356	-6.84410366630386	-3.99804643808576
H	-3.88639973405832	-6.58355800363170	-2.40405741105632
C	-5.97449346763744	-4.74192751323986	-4.16131024610504
H	-5.77804819986069	-3.97188138572445	-4.91694726180299
H	-6.89101645795144	-4.46370548109991	-3.63378002238259
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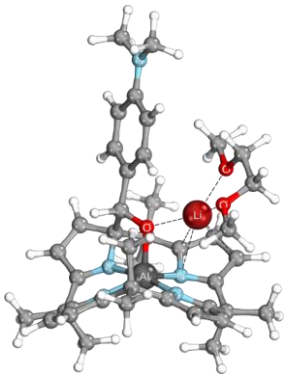

[**1**$^-$]-*p*-dimethylaminobenzaldehyde Li(dme) isomer A

N	-0.28822476186392	-2.31526317686536	0.04921846182205
C	-0.41949955931786	-3.58954285090142	0.53867194243575
C	0.36078830161668	-2.41775513917446	-1.15839416907434
C	0.13119129963583	-4.48511988368262	-0.34626099874325
H	0.17346148427080	-5.55686568867129	-0.23831164042998
C	0.63059463769546	-3.73488119513144	-1.43285849136425
H	1.13700620610880	-4.12494564321886	-2.30186941456945
N	-0.64374961526951	-1.54049214950809	2.65180540647331
C	-0.19430647029725	-0.94671079647490	3.80439141226937
C	-0.71831597360700	-2.89422045719920	2.89003593140784
C	-0.00742209366255	-1.90359380275765	4.77112190182524
C	-0.34642262125533	-3.14605093276702	4.18870242470704
H	-0.29927593973238	-4.11030847234146	4.66911764478187
C	-0.40806816606422	-0.28401455420122	-1.97500229341653
C	-2.11095749740882	0.88610018796610	-1.08296049021850
H	0.34919762172170	-2.13733170369944	-3.89789243005037
C	1.15597961125536	-1.60878108626917	-3.38969696548000
C	1.96075380299624	-0.48395554336294	-1.31570953104604
C	0.76819381830530	-1.21019584508069	-1.96849358861821
H	2.81657349809354	-1.15759714983273	-1.28621545579674
H	2.02265774827534	-2.26769122132770	-3.37142139396288
H	1.74500737925256	-0.18080606039105	-0.29125265280263
H	-3.19681188076627	-4.09366692951868	2.52113774086634
C	-2.66842024703896	-3.83165466242976	1.60108371680850
C	-0.80370814819195	-5.29613289608789	2.29315968692474
C	-1.14304105843020	-3.87858876487614	1.82960901918749
H	0.26592417967121	-5.41862214497907	2.45944000687158
H	-3.01616557967166	-2.85000200837282	1.28471471367350
H	-1.12280644766608	-6.02899800583599	1.55172221118309
H	0.35982336585298	2.06497109451087	5.37089908444610
C	0.08166691101007	1.01208496317482	5.30730639549763
C	1.61851656033495	0.69601843499544	3.37880420379962
C	0.16658091508414	0.51347195293928	3.86573201113168
H	1.90746561280505	1.74896011657246	3.39691437283135
H	0.76626617939956	0.45699901532093	5.94761597831605
H	1.74712574838402	0.33190158191051	2.35945101513021
C	-1.84039274785939	2.25659006788956	-0.37356133213718
C	-2.96730018910790	3.25074588633854	-0.64332069962171
C	-0.55018022895817	2.88508309952095	-0.93768745803467
H	-3.92808291698684	2.91510728265481	-0.26405337661465
H	-0.39186535350726	3.84672360598430	-0.44914873531987
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H	-0.61171313329464	3.06450630674781	-2.01288155761823
H	-3.07612395991271	3.43677224836256	-1.71299593266948
H	0.32954056031293	2.27777884119935	-0.73535792303001
H	2.24361254621572	0.40990013306704	-1.87719295290046
H	1.42974047504176	-0.73372743715703	-3.98220093477795
H	-1.32602991025671	-5.53212026739951	3.22090560755532
H	-2.95402433148753	-4.54846472173586	0.82898572335590
H	2.30140625427956	0.13372926578251	4.01668909723640
H	-0.92381368845039	0.89614628385440	5.71441676268074
H	0.35272189019538	-1.74478442878766	5.77566092535585
Al	-0.97237864693470	-0.74199697210102	0.95147833046050
C	-3.20403839890206	-0.10308820364590	-0.47894469376951
O	-2.79746347393668	-0.48180497209925	0.79682205574437
C	-2.16856074627623	0.97740573076924	-2.57367266481953
H	-2.89877081148523	1.53362559002747	-3.14038032367616
C	-1.15417822447842	0.27435108093665	-3.09504742796715
H	-0.92512549408029	0.12870729962082	-4.13911709550077
N	-0.93121434577694	0.08203904911074	-0.86436254083570
Li	-3.32357225789015	0.68623406085268	2.32901185907815
C	-0.73714837584092	1.33290212720879	2.99090458320125
C	-1.52673232087103	2.41132517576490	3.32677712136009
H	-1.65442266171062	2.84260000366936	4.30676141026532
C	-2.09522804907131	2.88353822958394	2.11880393687803
H	-2.72485305220406	3.75321134287840	2.01468185985033
C	-1.63164321683996	2.06844911733163	1.10935381335597
N	-0.80436905613669	1.10350042837455	1.64448475624226
O	-5.00070709745521	1.87064568698282	2.85232003733532
O	-4.11099670671820	-0.42939196978406	3.84235580917226
C	-5.81751773948905	1.19434063086710	3.77323253743887
H	-6.54298459180558	0.55764364452146	3.24962935002446
H	-6.38363097588712	1.90367234041372	4.39240560236619
C	-4.92708450202757	0.36656338074508	4.66206149783657
H	-5.55508044768336	-0.25420292670858	5.31492287678318
H	-4.31537147063858	1.01111068724264	5.30805646657803
C	-5.71385172694236	2.79394430299761	2.06287919372711
H	-4.99750368489220	3.31658424403671	1.43623256452630
H	-6.22706744472827	3.53073997591894	2.69071729226585
H	-6.44737899757129	2.29715249547740	1.42224571005030
C	-3.42957200848548	-1.44308681798032	4.56404834576318
H	-2.83449205495252	-2.01817713351047	3.86300655550561
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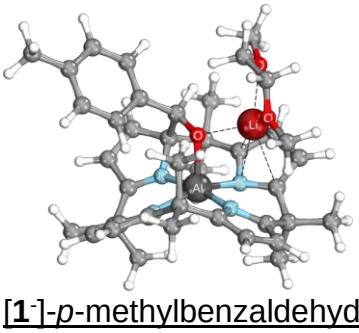
H	-2.75820046465858	-1.01934033627464	5.31392005629851
H	-3.12816389221891	-0.96851384479044	-1.16001863253698
C	-4.67270440041569	0.27486065046818	-0.48366667494657
C	-7.50828756432093	0.63772599659362	-0.55234853146024
C	-5.52105302476900	-0.37665028878483	0.41077768019689
C	-5.28893026760775	1.08710735106170	-1.42894210853390
C	-6.65937865737460	1.27728992761992	-1.46745973492611
C	-6.89412658403040	-0.20888424198575	0.38312870700499
H	-5.10770700541703	-1.06259905044426	1.13846770994749
H	-4.70385723276232	1.60422545192477	-2.17506362914374
H	-7.05898175199720	1.92739873177569	-2.23250204789232
H	-7.48591867468788	-0.76940405792409	1.09332735457544
N	-8.86900732334076	0.83655285403234	-0.56653460962719
C	-9.70820521202515	0.00763758417187	0.25865606279511
H	-9.46304494155148	0.12037036808637	1.31732144618828
H	-9.64192300700030	-1.05828959010488	0.01110807097181
H	-10.74517692448784	0.31270497760440	0.14076466906010
C	-9.46521301638281	1.53722104051489	-1.67398306633981
H	-9.08810752850486	2.55965393632661	-1.75007255741044
H	-10.53945750660020	1.60743044138414	-1.52142861312706
H	-9.29579337220627	1.04390760629457	-2.63826759184315



[**1**$^-$]-*p*-methylbenzaldehyde Li(dme) isomer B

N	0.10701365572291	-2.38927523502460	0.46956945842004
C	0.01598412696605	-3.61817087244370	1.07466781313587
C	0.65462388181426	-2.59470921350735	-0.77464712052406
C	0.48710416721251	-4.58760132135654	0.22063694589520
H	0.54583237803871	-5.64628419291147	0.41548955908945
C	0.89596269928437	-3.93261853794918	-0.96172106824275
H	1.33180880496228	-4.39617236095428	-1.83283853712750
N	-0.30241390480547	-1.34567077451374	2.97465666355123
C	0.17740743397025	-0.58498598399987	4.01386811260247
C	-0.17407354021965	-2.66502826119225	3.34782783600007
C	0.59234324701732	-1.40517897285402	5.03396785786663
C	0.36486117387013	-2.73310173098832	4.60854046094567
H	0.58364956353787	-3.62857883690103	5.16772315540619
C	-0.27813180530931	-0.61905575313326	-1.78641449631261
C	-2.03265255534475	0.49943070832288	-0.95635429595453
H	0.53528498081304	-2.60760814162055	-3.52898955602495
C	1.32758260450976	-1.98837251674841	-3.10777117809702
C	2.12037570552113	-0.59500015045731	-1.19736501328686
C	0.95997862582878	-1.46056571299583	-1.72427125136341
H	3.02131328347972	-1.20439175582252	-1.13295778333324
H	2.22999193297339	-2.59534067474429	-3.05105653795994
H	1.91884233497114	-0.20046119637866	-0.20162275977107
H	-2.53566235603144	-4.09753891877737	3.35334921438093
C	-2.11895381436504	-3.90644905616209	2.36136738925922
C	-0.07719169971621	-5.12038772193437	3.03965348238983
C	-0.58206635813152	-3.80198018043303	2.44910531328106
H	1.00928404820734	-5.13592754434367	3.11694197329688
H	-2.58215428929907	-3.00218232591766	1.97422525336020
H	-0.38872860553436	-5.96265883707346	2.42171042769397
H	0.22175684856245	2.60822314955303	5.29033929849856
C	0.13021455067018	1.52175034183269	5.32909029972693
C	1.68095966529574	1.29897303847168	3.39694275501001

C	0.28916299731033	0.91272882133583	3.93604389412662
H	1.78135977545335	2.38303721229944	3.31199871133635
H	0.90579388769155	1.15456561754956	6.00014061660346
H	1.86157338921152	0.86845231119090	2.41218967173474
C	-1.89771447709843	1.95975366029598	-0.41181143135793
C	-3.13042730673059	2.77894977707509	-0.79330058251302
C	-0.67159705779401	2.65251161811660	-1.02819739753094
H	-4.06221918153828	2.35290772017578	-0.42159197356019
H	-0.60954921408056	3.67053942058864	-0.64303892247551
H	-3.04977076422946	3.78878570292622	-0.39193869027217
H	-0.73688016264427	2.70965632943070	-2.11625555328724
H	-3.21498710064582	2.87636032189995	-1.87596800510933
H	0.25734817424016	2.15278275297495	-0.76133768967131
H	2.32223934291779	0.25066709780958	-1.85904169158362
H	1.53276981713371	-1.16796926255706	-3.79780949534504
H	-0.49718385300194	-5.28162380772384	4.03311648295772
H	-2.40456892401141	-4.73262657050843	1.70699527142580
H	2.45740911738730	0.92759706845459	4.06662425489964
H	-0.83526465109960	1.27209535589600	5.77091705420258
H	1.01982836585641	-1.09678731946677	5.97534954350212
Al	-0.72016897780725	-0.79130441165147	1.19091586152050
C	-3.10556514180453	-0.34103058346036	-0.15478208336049
O	-2.55904105094155	-0.76844978517669	1.05000037528315
C	-2.15396074914936	0.42803288932210	-2.44131255719965
H	-2.97290372605269	0.83596705807813	-3.01416549487229
C	-1.09139667743545	-0.22407914258081	-2.93062473279652
H	-0.88234282662545	-0.45964250248998	-3.96200955458086
N	-0.80153963773869	-0.19136144497362	-0.69659180117635
Li	-3.05329026322084	0.30019973387053	2.62338120072776
C	-0.75348717667509	1.47190618006009	3.01459570382611
C	-1.74443446829807	2.39491797640759	3.27495263880315
H	-1.96575076483700	2.85846245693886	4.22315875397773
C	-2.35947135464241	2.68429356180405	2.02949247637736
H	-3.13347426652045	3.41670876933483	1.85829784828615
C	-1.71236200283979	1.92304463538171	1.08139495440416
N	-0.74793566868216	1.14785919317378	1.68496404593096
O	-5.12261512224264	0.57859392037127	2.55553385182939
O	-3.63001845541587	-0.97237711350773	4.05006957032937
C	-5.59061572152694	-0.74136627636188	2.74843560196509
H	-5.29461294030036	-1.37785987022631	1.90538422099724
H	-6.68511279305742	-0.76682635447490	2.82151239547834
C	-5.00577151311310	-1.24268610636834	4.04709012527959
H	-5.19946633400551	-2.31961962005251	4.13591653737457
H	-5.49301654216858	-0.74629665081631	4.89788211842173
C	-5.91726078314506	1.34759505033465	1.68870941238516
H	-5.44066732348048	2.31953142294875	1.58047536950943
H	-6.92278496875316	1.49242424345022	2.09747030107001
H	-6.01312564539221	0.88881214138267	0.69802102013036
C	-2.97185620172498	-1.45804429780710	5.20377752535412
H	-1.92406239872182	-1.17701425341212	5.14440312625116
H	-3.03496499141373	-2.54795551926505	5.25851767545473
H	-3.41217613084246	-1.02933807599969	6.11099512509649
H	-3.94529511678826	0.34105699972163	0.03415676290651
C	-3.64769835727971	-1.47685641198068	-0.99135365051779
C	-4.66485872602682	-3.50333740718814	-2.66520071040981
C	-3.00181691940439	-2.70526395796080	-1.09153998242917
C	-4.81274572398856	-1.28574631553285	-1.72378331692559
C	-5.31458239941267	-2.28033300425877	-2.55021576012991
C	-3.50374268603100	-3.69446961276635	-1.92010667730309
H	-2.10192984100635	-2.90876185190357	-0.52812930367593
H	-5.34175650229647	-0.33985177485685	-1.65389109667813
H	-6.22686663591927	-2.10271609437761	-3.10767990569994
H	-2.97315025445516	-4.63745389545310	-1.98317384938435
C	-5.20221341928394	-4.59598682694644	-3.54253434767601
H	-4.42794448441964	-5.00053174729940	-4.19537009296626
H	-6.01574095780360	-4.24200972229001	-4.17485421500979
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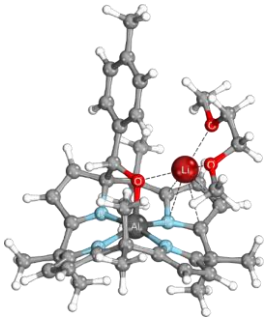

[**1**$^{-}$]-*p*-methylbenzaldehyde Li(dme) isomer A

N	-0.20998517114460	-2.29778538545707	0.03897937915237
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C	0.44735097543886	-2.36775114845021	-1.16647149177501
C	0.28433460695969	-4.44849929056318	-0.37255187053262
H	0.36275081928009	-5.51906434559173	-0.27345077511544
C	0.76245988659309	-3.67260523497646	-1.45075727342929
H	1.28592875167535	-4.03805066457723	-2.32034028646799
N	-0.60450099869606	-1.55519821229637	2.64475640659513
C	-0.18006131061073	-0.95448101968361	3.80358730605267
C	-0.63282177192913	-2.91256632631509	2.87282708445704
C	0.03581209041832	-1.91145798827493	4.76398002754980
C	-0.25770344136421	-3.16063763895529	4.17117465505214
H	-0.17932876285143	-4.12611769665257	4.64495018219157
C	-0.38787637013248	-0.25431805828245	-1.96873264707225
C	-2.13764977967796	0.84760583882308	-1.07877481598834
H	0.44702064326484	-2.06032659466891	-3.90357687704031
C	1.23170551192833	-1.51043964786603	-3.38355022756203
C	1.98157497293718	-0.37927513702359	-1.29223278420878
C	0.81982459652867	-1.13918006812810	-1.96175542115479
H	2.85942144586020	-1.02385834253219	-1.26181475297291
H	2.11948106232784	-2.14060590416390	-3.36468583934201

H	1.74774579715403	-0.09353042637942	-0.26672009765206
H	-3.06696258634324	-4.19228362140770	2.48393489375403
C	-2.54329075429973	-3.90775473621358	1.56798317988310
C	-0.63114849976362	-5.31149636243688	2.25819409080485
C	-1.01822693716637	-3.90343279272391	1.80333927448206
H	0.44137633337690	-5.39715224139733	2.42884892672329
H	-2.92259582247891	-2.93697838146507	1.25438594328560
H	-0.92046886270842	-6.04960023359738	1.50981738761514
H	0.27772526546599	2.06205963264978	5.39253561240093
C	0.03157354567776	1.00176433317065	5.32096235825372
C	1.58029194134021	0.74834855991460	3.39300044242659
C	0.13390049385676	0.51610390142873	3.87604125514975
H	1.83556577943788	1.80978825278581	3.41926478388166
H	0.73210098427470	0.46326453664119	5.95813983865511
H	1.72225754505806	0.39590602018579	2.37130541263773
C	-1.92245714241292	2.22076613914235	-0.35654085989637
C	-3.08942084010992	3.16953893435947	-0.61896730237380
C	-0.65815808782093	2.90492495877722	-0.91395840309730
H	-4.03456752655498	2.79220141376497	-0.23929269795811
H	-0.53561196788155	3.86529258683112	-0.41299254587500
H	-2.89687488318569	4.13629722828593	-0.15398852045869
H	-0.72818358320793	3.09562334512795	-1.98663870444244
H	-3.20845500435810	3.35802911217140	-1.68703095335873
H	0.24405245346157	2.32849964805376	-0.72049403126314
H	2.23861915647048	0.52899561824213	-1.84286600746295
H	1.48123904507674	-0.62105504636527	-3.96533003259095
H	-1.14907106476371	-5.57285177309237	3.18156959925361
H	-2.80082929732070	-4.62977576552911	0.79092322700837
H	2.27988398072502	0.20365559363458	4.02797737158640
H	-0.97010133691618	0.85241379371379	5.72643744739654
H	0.38668986136475	-1.74800980179374	5.77103036315487
Al	-0.95099090505892	-0.75748224853692	0.94910896624380
C	-3.19768626974930	-0.18372515380079	-0.48800108951028
O	-2.78509751631262	-0.55862484108149	0.78471779799185
C	-2.18732157541156	0.95001261077977	-2.56973691200901
H	-2.92998947262775	1.48721096171111	-3.13855062161768
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C	-1.70826178862549	2.03015676397171	1.12559117834476
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O	-4.09910587312186	-0.56237966142509	3.83273433300570
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H	-6.55954297405769	0.35007157287484	3.24115554651616
H	-6.44668286868443	1.69332008613856	4.39161158212940
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H	-6.50581352042729	2.11978997948822	1.41610473521814
C	-3.39469461160834	-1.56431069367600	4.54955406092165
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H	-4.09865518205805	-2.24800408327849	5.03502568657950
H	-2.73473579526724	-1.12904793965846	5.30274731627596
H	-3.09456785186465	-1.03947927919793	-1.17830670939750
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H	-4.73706202268393	1.45298758443518	-2.20504041804742
H	-7.13884211545049	1.68524768414881	-2.25946060821528
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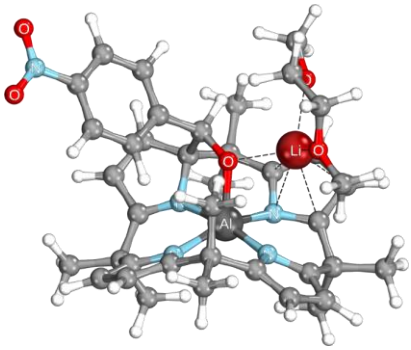
H	-9.31216752055348	1.56943936491234	-0.58433644113773
H	-9.48391547599429	-0.01264399132516	0.16638538059746
H	-9.39680015684363	0.12874945495240	-1.58305570417196



[**1**$^{-}$]-*p*-nitrobenzaldehyde Li(dme) isomer B

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C	0.37137311398656	-4.60080758137255	0.15045731352405
H	0.40018797166416	-5.66369443143007	0.32801246976823
C	0.78934809102731	-3.94048961165119	-1.02586935782235
H	1.20253541798730	-4.40444447618145	-1.90765861733902
N	-0.32792509209768	-1.37040757386601	2.95118709804057

C	0.16323183984776	-0.62381637110527	3.99577884479364
C	-0.21201205143272	-2.69480121340672	3.31176997480496
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C	0.32996522049336	-2.77931524646483	4.56995840367105
H	0.54064344079126	-3.68180173465187	5.12080383881782
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C	-2.04350187344697	0.52791781190308	-0.96179565328785
H	0.49292862036722	-2.57271432753554	-3.57131040158843
C	1.29262402442692	-1.97290455325250	-3.13615297810705
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C	0.92709921640033	-1.45798521776605	-1.74741122885299
H	2.98816246772351	-1.24722580094992	-1.13941266545158
H	2.18386088291446	-2.59628164782741	-3.08263117458191
H	1.89973399472778	-0.23310311368193	-0.20331964524052
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C	-0.64048974249311	-3.81952736874046	2.40713046590559
H	0.94661395400420	-5.17378937466879	3.04314750015997
H	-2.63860266050374	-2.99662849665176	1.96709676098444
H	-0.46702911298744	-5.98188179383635	2.35802850926020
H	0.25700094455154	2.55974874224365	5.29394141876260
C	0.15213062304057	1.47433052194548	5.32689676126531
C	1.68626239638422	1.24547857279169	3.38302573637176
C	0.29322020296957	0.87285824751272	3.92883774498114
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H	1.85550399628964	0.82110094870435	2.39348553996365
C	-1.90322257019081	1.98031498760001	-0.39864776785258
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C	-0.67411688718737	2.67372165368567	-1.00854745371740
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H	-0.60574644788631	3.68592688454977	-0.60968507218709
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H	-0.74053110165232	2.74650325883628	-2.09556120198337
H	-3.21304344747267	2.92554430428694	-1.85160457126268
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H	1.51620443625676	-1.14677342597865	-3.81339684526012
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H	-2.48214613209744	-4.72848494489628	1.68424716354291
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H	-0.81238746368143	1.23381378437235	5.77575998591326
H	1.00591724336126	-1.16236547926229	5.94951821345821
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C	-2.16186752623081	0.47713562923204	-2.44884284509325
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H	-1.93421972172767	2.84678726971260	4.24229412244871
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O	-3.65582577303670	-0.96095862792301	4.03611061473370
C	-5.63087608165310	-0.66851033297862	2.76992098758529
H	-5.37027294969876	-1.32514740517337	1.93041439667533
H	-6.72409242871779	-0.65688130076201	2.86048935288962
C	-5.04143332507186	-1.17540014546978	4.06376252514389
H	-5.27646301218654	-2.24216259148106	4.17233333670377
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C	-5.90994566951465	1.42365458618885	1.70093233685168
H	-5.40790229866446	2.38137048660196	1.58286391521337
H	-6.90322537694620	1.59726307375993	2.12736486372718
H	-6.03760539448178	0.96763003833327	0.71226006382659
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H	-3.11599234448852	-2.54002855378964	5.26598849908537
H	-3.39879984041938	-0.98832960830512	6.09365933433066
H	-3.96592085134676	0.35518790689859	0.01900218972457
C	-3.64382073941264	-1.44853091383624	-1.02560347167974
C	-4.61350629588634	-3.43244861152899	-2.69969270936584
C	-3.00105108001777	-2.67932861417563	-1.10309998172537
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H	-6.17957235706256	-2.05168386027980	-3.20881362516163
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O	-4.51347979216014	-5.51569459663496	-3.63090739055487
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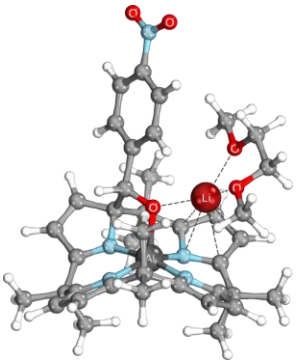

[**1**$^-$]-*p*-nitrobenzaldehyde Li(dme) isomer B

N	-0.19681035729429	-2.30289246953184	0.03823008225780
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C	-2.15566623516718	0.81694051781902	-1.10066276225892
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C	0.83066460686104	-1.13730462442215	-1.96003875746546
H	2.86382023604162	-0.99327107977220	-1.24857633760664
H	2.15211346616491	-2.12503787954202	-3.35117921179406
H	1.73586839482750	-0.07354689690541	-0.26254639681889
H	-3.04361469354299	-4.23293835020000	2.46746307937394
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C	-0.99364540429668	-3.91383417009883	1.80279548525805
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C	-0.03888445638171	1.01726788301751	5.31177848667739
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H	1.77771002164305	1.83898383344794	3.42578284622487
H	0.65773000717545	0.48661024300994	5.95947143381439
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C	-0.69608876890762	2.88931614503485	-0.94544779975469
H	-4.07527503442418	2.75253427744386	-0.28145151013727
H	-0.58267079014841	3.85255044768832	-0.44810734935922
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H	-3.24786534678324	3.31211143180890	-1.73141824340414
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H	-1.04459719840422	0.86060586918918	5.70466215410740
H	0.36258299689597	-1.72670423567906	5.76953789312762
Al	-0.95963988665538	-0.77188631472667	0.93970267290474
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H	-0.89321040373346	0.13629752640350	-4.14522037600375
N	-0.94500116040758	0.06340139518677	-0.87123750095796
Li	-3.28684404349068	0.57780163946544	2.36151737943801
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H	-1.79707162170098	2.81156219164016	4.28912155748452
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C	-1.74411645559918	2.01888046878665	1.09691791212903
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O	-5.05437643285667	1.68809302245916	2.86241559783333
O	-4.08946607773149	-0.58452842434659	3.83651102395189
C	-5.82495837514796	1.01222621989609	3.82428121521003
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H	-6.37309814368393	1.72042939924072	4.45977505480105
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H	-5.48922862078811	-0.43015256689681	5.35468408624959
H	-4.26909753698913	0.85300122324366	5.30867290882069
C	-5.80264520146699	2.62452314489208	2.12512201262828
H	-5.12608127789220	3.12906221627381	1.44191118406650
H	-6.25425978179507	3.37470671598080	2.78288296903260
H	-6.59691271700516	2.14444303597240	1.54544999624182
C	-3.41530035572684	-1.62412763191111	4.52999548013548
H	-2.82005025623217	-2.18001888002464	3.81391031649946
H	-4.14013711855870	-2.29804976455586	4.99774059089387
H	-2.74397036477690	-1.22671386018400	5.29378095966934
H	-3.11172191276050	-1.07351125537518	-1.19377402004019
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C	-7.46623760119512	0.37296094137172	-0.57149376481390
C	-5.49849329292025	-0.53604619035077	0.43126427934463
C	-5.32413845424673	0.84668274765039	-1.50717488964131
C	-6.69868619319745	0.99814171243365	-1.53910906659723
C	-6.87537144615097	-0.40323474925105	0.41109310929558
H	-5.04776881745697	-1.16196328683895	1.18812111762617
H	-4.74972494916484	1.33893910060405	-2.27578484098562
H	-7.16273022981995	1.59474167107398	-2.31069236686122
H	-7.47987234547330	-0.91166509025731	1.14828737266801
N	-8.91607282404511	0.53459325820549	-0.58788555104103
O	-9.54313031350473	0.02229208512141	0.30687873104429
O	-9.39550646200945	1.17593879891254	-1.49018593822112

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