# Electronic Supporting Information

# Synthesis, characterization and reactivity of an imidazolin-2-iminato aluminium dihydride

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## Crystallographic data of 2-8

**Table S1** Crystallographic data of **2-5**.

| | **2** | **3**$(THF)_3$ | **4**$(toluene)_{1.5}$ | **5**$(toluene)_{1.5}$ |
|---|---|---|---|---|
| Formula | $C_{54}H_{76}Al_2N_6$ | $C_{68}H_{98}Al_2F_6N_6O_9S_2$ | $C_{129}H_{200}Al_4B_8N_{12}$ | $C_{129}H_{168}Al_4Br_8N_{12}$ |
| $F_w$ | 863.17 | 1375.60 | 2113.41 | 2633.95 |
| Colour, shape | Colourless, block | Colourless, block | Colourless, plate | Colourless, prism |
| Temp. (K) | 150(2) | 150(2) | 150(2) | 150(2) |
| Cryst. syst. | Monoclinic | Monoclinic | Monoclinic | Monoclinic |
| Space group | $P2_1/c$ | $P2_1/c$ | $C2/c$ | $C2/c$ |
| $a$ (Å) | 16.5406(1) | 26.3370(8) | 48.7528(13) | 48.620(2) |
| $b$ (Å) | 14.2392(1) | 12.1672(3) | 12.0476(3) | 12.090(1) |
| $c$ (Å) | 22.0959(1) | 25.4631(8) | 22.9213(5) | 22.859(1) |
| $\alpha$ (°) | 90 | 90 | 90 | 90 |
| $\beta$ (°) | 90.9867(4) | 118.280(4) | 105.547(3) | 106.432(7) |
| $\gamma$ (°) | 90 | 90 | 90 | 90 |
| $V$ (Å$^3$) | 5203.37(4) | 7185.7(4) | 12970.3(6) | 12888.4(12) |
| $Z$ | 4 | 4 | 4 | 4 |
| $D_{calcd.}$ (g cm$^{-3}$) | 1.102 | 1.272 | 1.082 | 1.357 |
| $F$(000) | 1872 | 2928 | 4600 | 5432 |
| $\mu$ (mm$^{-1}$) | 0.798 | 1.521 | 0.087 | 2.568 |
| Cryst. size (mm$^3$) | 0.56 × 0.36 × 0.31 | 0.52 × 0.38 × 0.23 | 0.34 × 0.16 × 0.08 | 0.40 × 0.37 × 0.20 |
| Reflections collected | 36966 | 27594 | 48749 | 46122 |
| Indep. Reflns ($R_{int}$) | 9324 (0.0230) | 12943 (0.0355) | 12943 (0.0730) | 11336 (0.0810) |
| Data/restraints/params | 9324/119/646 | 12943/618/1022 | 12943/585/865 | 11336/861/801 |
| GOOF on $F^2$ | 1.009 | 1.372 | 1.016 | 1.072 |
| $R_1$, w$R_2$ ($I$> 2$\sigma$($I$)) | 0.0493, 0.1252 | 0.0928, 0.2238 | 0.0529, 0.1366 | 0.0499, 0.0739 |
| $R_1$, w$R_2$ (all data) | 0.0516, 0.1272 | 0.1129, 0.2386 | 0.0688, 0.1514 | 0.0843, 0.0815 |
| Largest diff peak and hole (e Å$^{-3}$) | 0.755 and −0.659 | 1.614 and −1.155 | 0.521 and −0.329 | 0.477 and −0.498 |

**Table S2** Crystallographic data of **6**, **7**, and **8**.

| | **6**(toluene)$_{1.5}$ | **7**(THF)$_6$ | **8**(toluene) |
|---|---|---|---|
| Formula | $C_{129}H_{168}Al_4Cl_8N_{12}$ | $C_{78}H_{120}Al_2I_4N_6O_6$ | $C_{61}H_{80}Li_2N_6$ |
| $F_w$ | 2278.27 | 1799.36 | 911.19 |
| Colour, shape | Colourless, block | Colourless, block | Yellow, plate |
| Temp. (K) | 150(2) | 150(2) | 150(2) |
| Cryst. syst. | Monoclinic | Monoclinic | Triclinic |
| Space group | *C*2/*c* | *C*2/*c* | *P*–1 |
| *a* (Å) | 48.612(2) | 22.3083(5) | 11.115(1) |
| *b* (Å) | 12.0883(4) | 16.8446(3) | 14.879(1) |
| *c* (Å) | 22.579(1) | 24.0034(5) | 17.490(1) |
| *α* (°) | 90 | 90 | 81.656(5) |
| *β* (°) | 105.956(6) | 114.736(3) | 80.281(5) |
| *γ* (°) | 90 | 90 | 82.250(6) |
| *V* (Å$^3$) | 12756.8(8) | 8192.3(3) | 2802.6(3) |
| *Z* | 4 | 4 | 2 |
| $D_{calcd.}$ (g cm$^{-3}$) | 1.186 | 1.459 | 1.080 |
| *F*(000) | 4856 | 3664 | 988 |
| *μ* (mm$^{-1}$) | 0.256 | 12.558 | 0.062 |
| Cryst. size (mm$^3$) | 0.73 × 0.44 × 0.21 | 0.50 × 0.32 × 0.30 | 0.28 × 0.20 × 0.10 |
| Reflections collected | 52472 | 16135 | 20755 |
| Indep. Reflns ($R_{int}$) | 11220 (0.0816) | 7374 (0.0479) | 9860 (0.0834) |
| Data/restraints/params | 11220/243/731 | 7374/0/443 | 9860/168/702 |
| GOOF on $F^2$ | 1.037 | 1.062 | 1.063 |
| $R_1$, w$R_2$ ($I > 2\sigma(I)$) | 0.0585, 0.1123 | 0.0643, 0.1799 | 0.0840, 0.1389 |
| $R_1$, w$R_2$ (all data) | 0.0906, 0.1261 | 0.0695, 0.1822 | 0.1524, 0.1672 |
| Largest diff peak and hole (e Å$^{-3}$) | 0.472 and −0.320 | 1.682 and −1.598 | 0.306 and −0.240 |

## Molecular structures of 6, 7, and 8 in the solid state

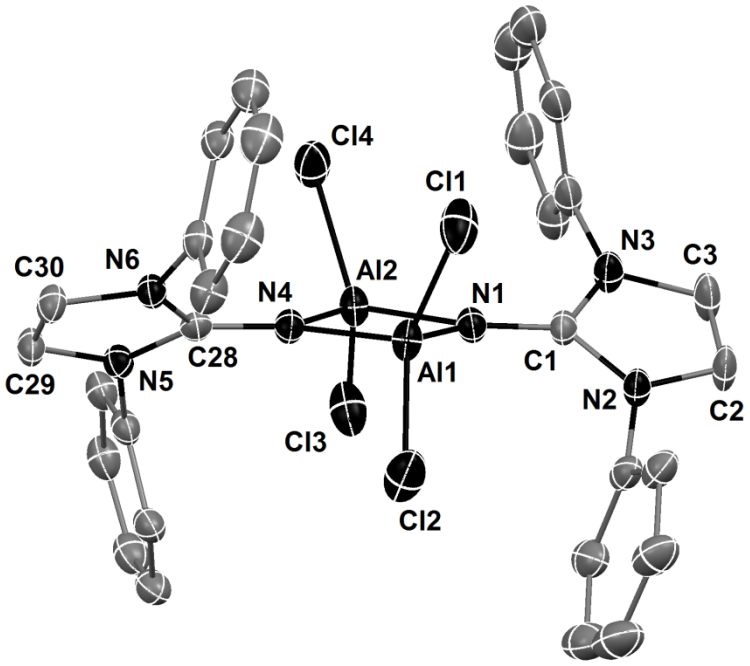


**Fig. S1** Molecular structure of **6**(toluene)$_{1.5}$ in the solid state. Hydrogen atoms, isopropyl groups, and toluene molecules have been omitted for clarity; displacement ellipsoids are drawn at the 50% probability level. Selected bond lengths (Å), atom···atom distance (Å), and bond angles (°): Al(1)–Cl(1) 2.141(1), Al(1)–Cl(2) 2.122(1), Al(1)–N(1) 1.871(2), Al(1)–N(4) 1.867(2), Al(2)–Cl(3) 2.124(1), Al(2)–Cl(4) 2.141(1), Al(2)–N(1) 1.861(2), Al(2)–N(4) 1.873(2), N(1)–C(1) 1.320(3), N(2)–C(1) 1.380(3), Al(1)···Al(2) 2.693(1); Cl(1)–Al(1)–Cl(2) 109.99(5), N(1)–Al(1)–N(4) 87.7(1), N(1)–Al(2)–N(4) 87.8(1), Al(1)–N(1)–Al(2) 92.3(1), Al(1)–N(1)–C(1) 134.9(2), Al(2)–N(1)–C(1) 132.8(2), Al(1)–N(4)–Al(2) 92.1(1).

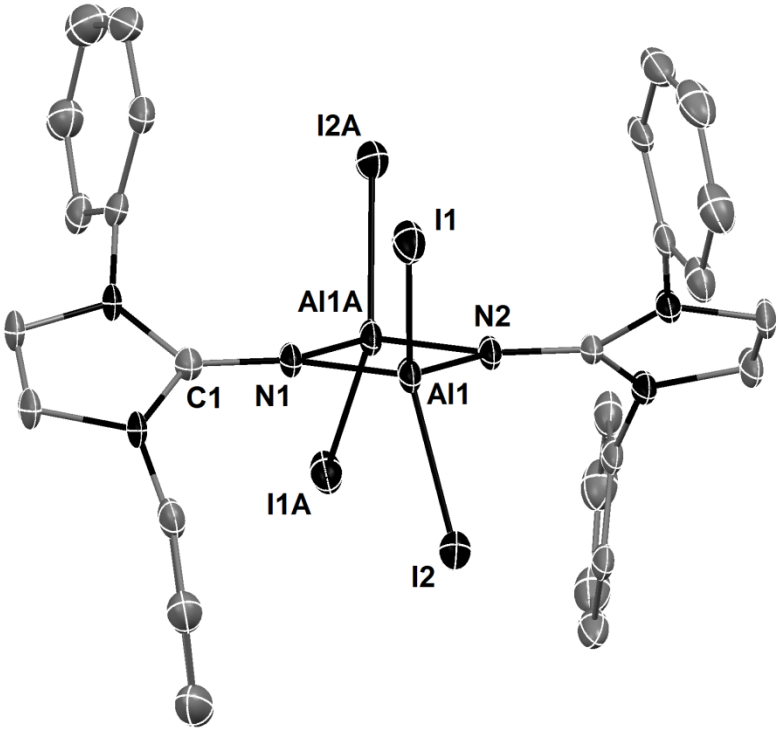


**Fig. S2** Molecular structure of **7**$(THF)_6$ in the solid state. Hydrogen atoms, isopropyl groups, and THF molecules have been omitted for clarity; displacement ellipsoids are drawn at the 50% probability level. Selected bond lengths (Å), atom···atom distance (Å), and bond angles (°): I(1)–Al(1) 2.541(2), I(2)–Al(1) 2.543(2), Al(1)–N(1) 1.871(6), Al(1)–N(2) 1.874(6), N(1)–C(1) 1.335(13), Al(1)···Al(1A) 2.688(4); I(1)–Al(1)–I(2) 107.6(1), N(1)–Al(1)–N(2) 88.2(3), Al(1)–N(1)–Al(1A) 91.8(4), Al(1)–N(1)–C(1) 134.1(2), Al(1A)–N(1)–C(1) 134.1(2), Al(1)–N(2)–Al(1A) 91.7(4). Symmetry transformation used to generate equivalent atoms: A: −x+1, y, −z+0.5.

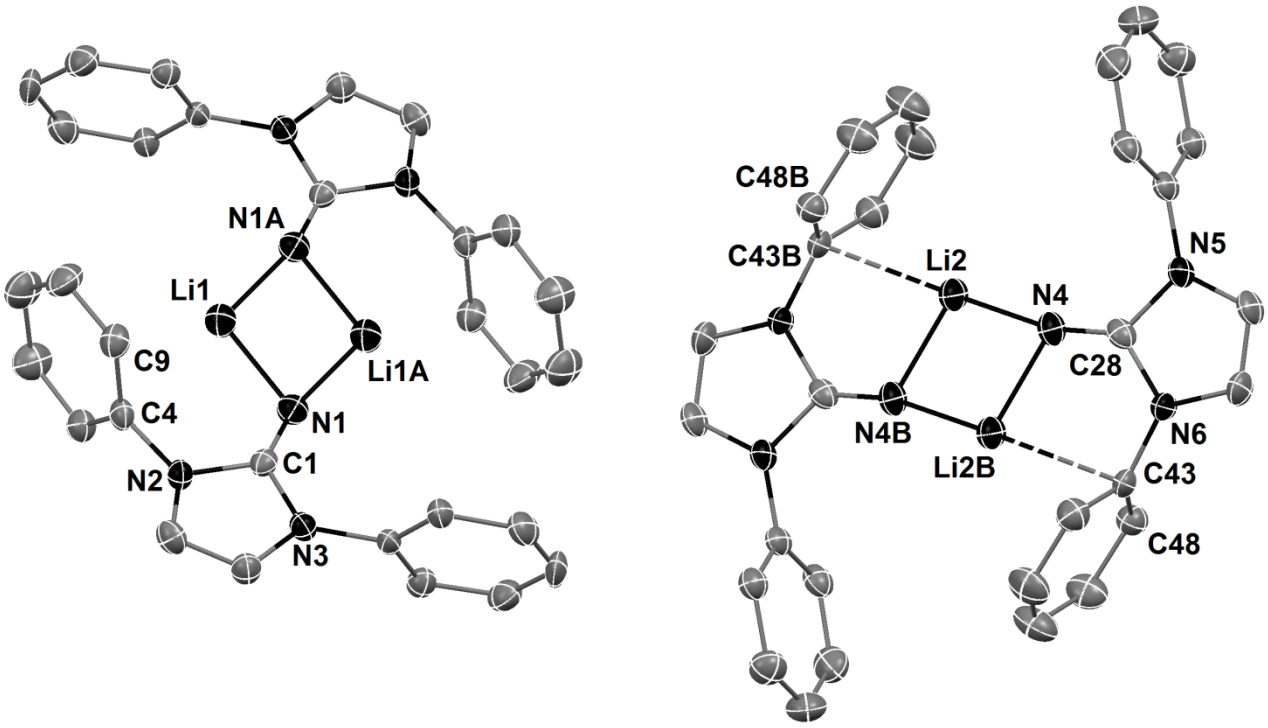


**Fig. S3** Molecular structure of **8**(toluene) in the solid state. The asymmetric unit consists of two centrosymmetric dimers. Hydrogen atoms, isopropyl groups, and toluene molecules have been omitted for clarity; displacement ellipsoids are drawn at the 50% probability level. Selected bond lengths (Å), atom···atom distances (Å), and bond angles (°): N(1)–C(1) 1.241(3), N(1)–Li(1) 1.981(6), N(1A)–Li(1) 1.852(5), N(4)–Li(2) 1.841(6), Li(2)–N(4B) 1.992(6), C(4)···Li(1) 2.610(6), C(9)···Li(1) 2.738(6), C(43B)···Li(2) 2.548(6), C(48B)···Li(2) 2.721(7), Li(1)···Li(1A) 2.387(11), Li(2)···Li(2B) 2.366(11); C(1)–N(1)–Li(1) 119.3(3), C(1)–N(1)–Li(1A) 160.2(3), Li(1)–N(1)–Li(1A) 77.0(3), N(1)–Li(1)–N(1A) 103.0(3), C(28)–N(4)–Li(2) 166.0(3), C(28)–N(4)–Li(2B) 117.9(3), Li(2)–N(4)–Li(2B) 76.1(3), N(4)–Li(2)–N(4B) 103.9(3). Symmetry transformations used to generate equivalent atoms: A: −x, −y+1, −z+1; B: −x+1, −y+2, −z.

**Synthetic procedures: General considerations**

All experiments and manipulations were carried out under dry oxygen-free nitrogen using standard Schlenk techniques or in an MBraun drybox containing an atmosphere of purified nitrogen. Glass junctions were coated with the PTFE-based grease Merkel Triboflon III. Solvents were dried by standard methods and freshly distilled prior to use. NMR spectra were recorded on Bruker Avance 400 or Avance III 500 spectrometers. Chemical shift values are referenced to (residual) solvent signals ($^{1}$H- and $^{13}$C{$^{1}$H} NMR). *J* coupling values are reported in Hz. Abbreviations: s = singlet, d = doublet, m = multiplet, Dipp = 2,6-diisopropylphenyl, L = bis(2,6-diisopropylphenyl)imidazolin-2-imino. High resolution mass spectra were recorded on a Thermo Fisher Scientific LTQ Orbitrap XL using an APCI ion source and providing the analyte dissolved in toluene. Reagents purchased from commercial sources were used as received if not stated otherwise. Boron tribromide was stored over mercury.

**Procedures for the synthesis of {$\mu$-LAlX$_2$}$_2$ (5, X = Br; 6, X = Cl) *via* conversion of {$\mu$-LAlH$_2$}$_2$ (2) with BX$_3$ (X = Br, Cl) and respective NMR spectra**

**Synthesis of {$\mu$-LAlBr$_2$}$_2$ (5)** In a Schlenk tube equipped with a magnetic stirrer bar and a rubber septum a solution of {$\mu$-LAlH$_2$}$_2$ (**2**; 0.157 g, 0.18 mmol) in toluene (2 mL) was cooled to −78 °C. Under stirring, 1.47 g (1.5-1.6 mL, 0.37 mmol) of a solution of boron tribromide in toluene (prepared as a mixture of 1.35 g $BBr_3$ in 19.11 g toluene and assumed as 0.24 M) was added dropwise *via* syringe (gradually over a period of 2-3 min). The septum was exchanged for a glass stopper and the reaction mixture was left in the cooling bath to stir over night while warming to room temperature. The connection to the inert-gas system was maintained to prevent build-up of pressure. From the resulting colourless suspension the volatiles were removed under reduced pressure and the solid residue was dried *in vacuo* ($9\cdot10^{-2}$ mbar, 2 h). Yield: quantitative ($^{1}$H NMR-spectroscopic control, *cf.* Fig. S4). The formation of **5** was verified by high resolution mass spectrometry: HRMS: *m/z* found, (calc.): 1179.21987 $[M + H]^+$ (68%), (1179.22201).

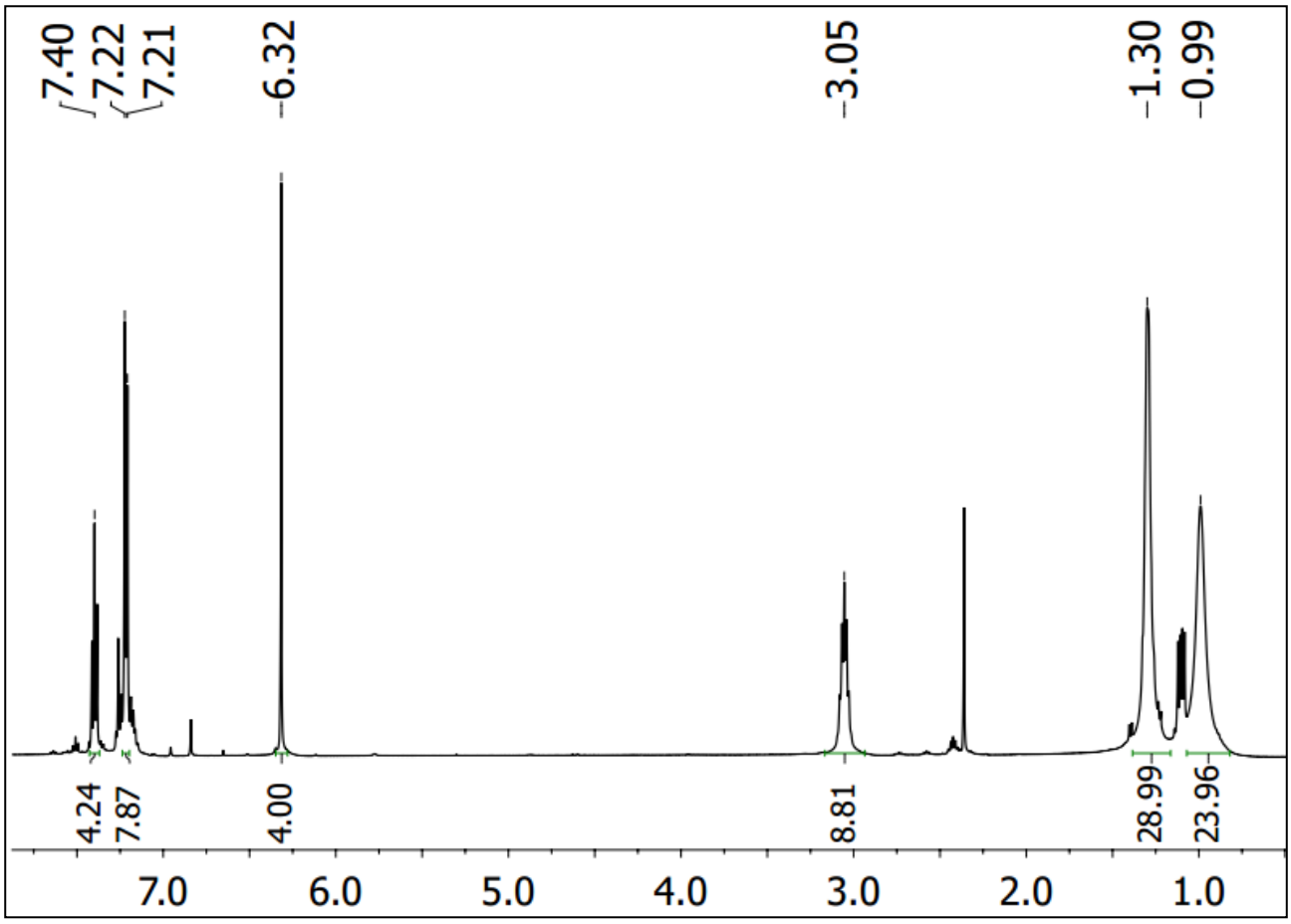


**Fig. S4** $^{1}$H NMR spectrum (400.1 MHz, $CDCl_3$) of crude **5** as obtained *via* conversion of **2** with 2 eq $BBr_3$ in toluene.

**Synthesis of $\{\mu\text{-LAlCl}_2\}_2$ (6)** In a Schlenk tube equipped with a magnetic stirrer bar and a rubber septum a solution of $\{\mu\text{-LAlH}_2\}_2$ (**2**; 0.236 g, 0.28 mmol) in toluene (4 mL) was cooled to −78 °C. Under stirring, 0.46 g (0.62 mL, 0.62 mmol) of a solution (1 M) of boron trichloride in hexane was added dropwise *via* syringe (gradually over a period of 1-2 min). The septum was exchanged for a glass stopper and the reaction mixture was left in the cooling bath to stir over night while warming to room temperature. The connection to the inert-gas system was maintained to prevent build-up of pressure. From the resulting colourless suspension the volatiles were removed under reduced pressure. From the $^1$H NMR data of a sample we concluded 60% conversion to **6**. The solid residue was redissolved in toluene (4 mL) and under ice-cooling and stirring another 0.6 mL of the $BCl_3$ solution (*vide supra*) was added. After 1 h, the ice bath was removed and stirring continued over night. The solvent was evaporated under reduced pressure and the solid dried *in vacuo* ($9\cdot10^{-2}$ mbar, 2 h). Yield: 80-85% as estimated from the $^1$H NMR analysis (*cf.* Fig. S5, Fig. S6). The formation of **6** was verified by high resolution mass spectrometry: HRMS: *m/z* found, (calc.): 1001.42351 $[M + H]^+$ (63%), (1001.42521).

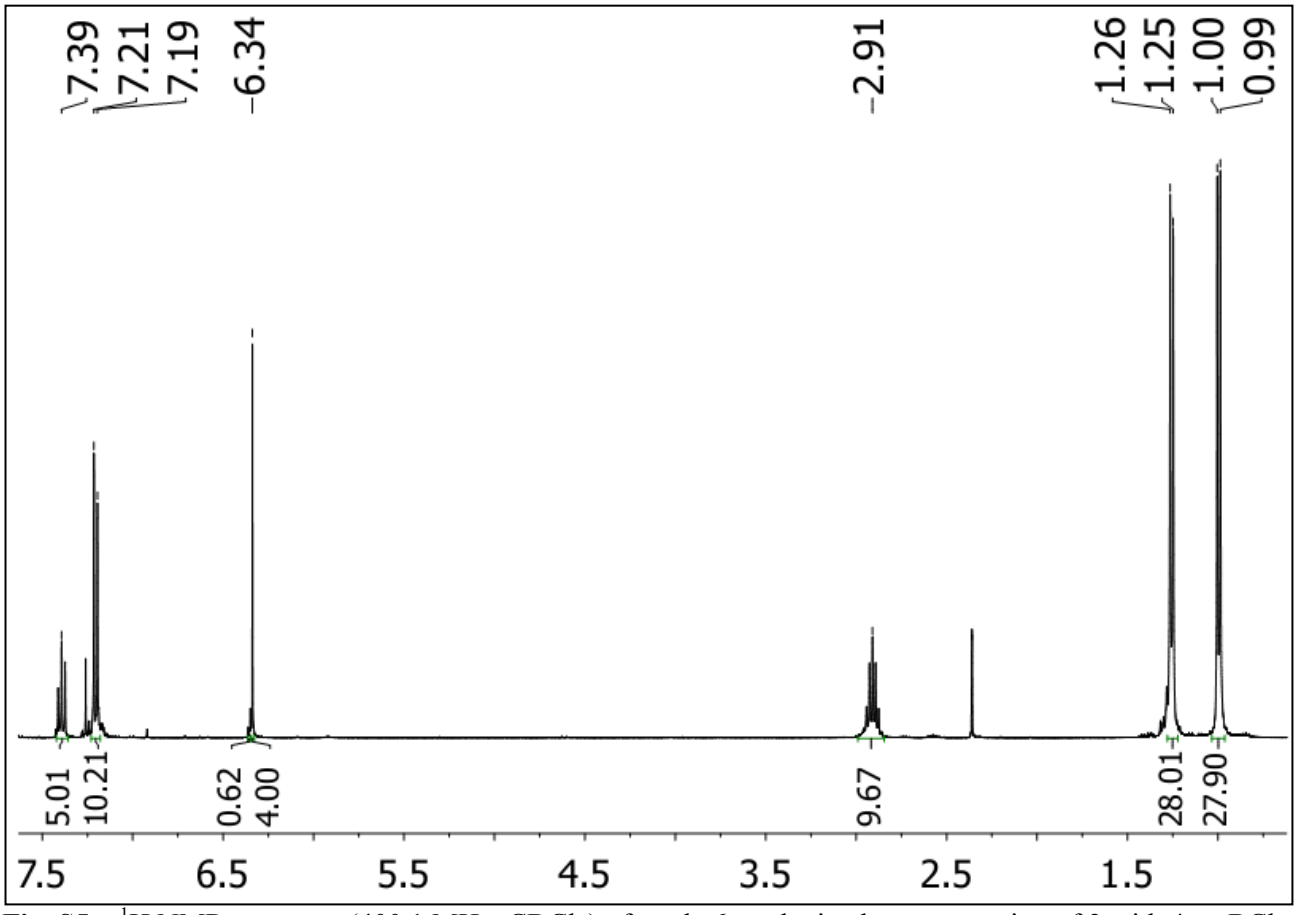


**Fig. S5** $^{1}$H NMR spectrum (400.1 MHz, $CDCl_3$) of crude **6** as obtained *via* conversion of **2** with 4 eq $BCl_3$ in toluene.

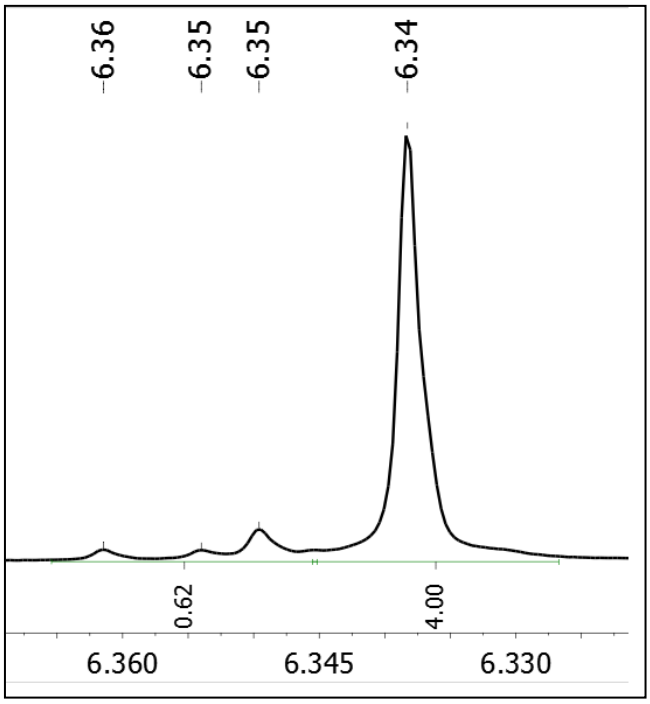


**Fig. S6** Expansion of the imidazolin-C*H* region of the $^{1}$H NMR spectrum shown in **Fig. S5**; relevant for the determination of the product-to-side-product-ratio).

**$^{1}$H- and $^{13}$C NMR spectra of crude 6 as obtained *via* conversion of {LLi}$_2$ (8) with 2 eq AlCl$_3$**

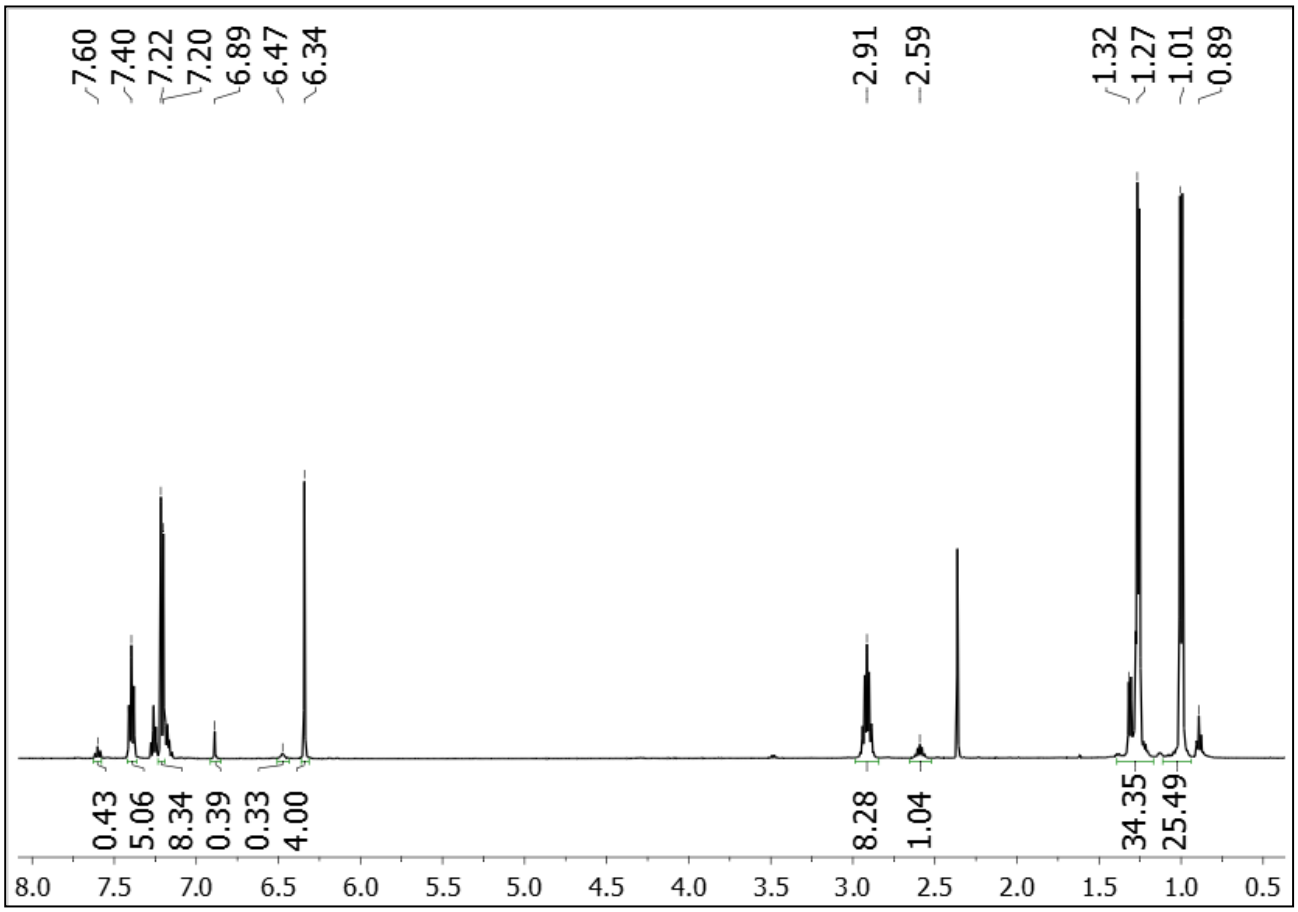


**Fig. S7** $^{1}$H NMR spectrum (500.1 MHz, $CDCl_3$) of crude **6** as obtained *via* conversion of {LLi}$_2$ (**8**) with 2 eq $AlCl_3$ in toluene (*cf.* Experimental section in main article).

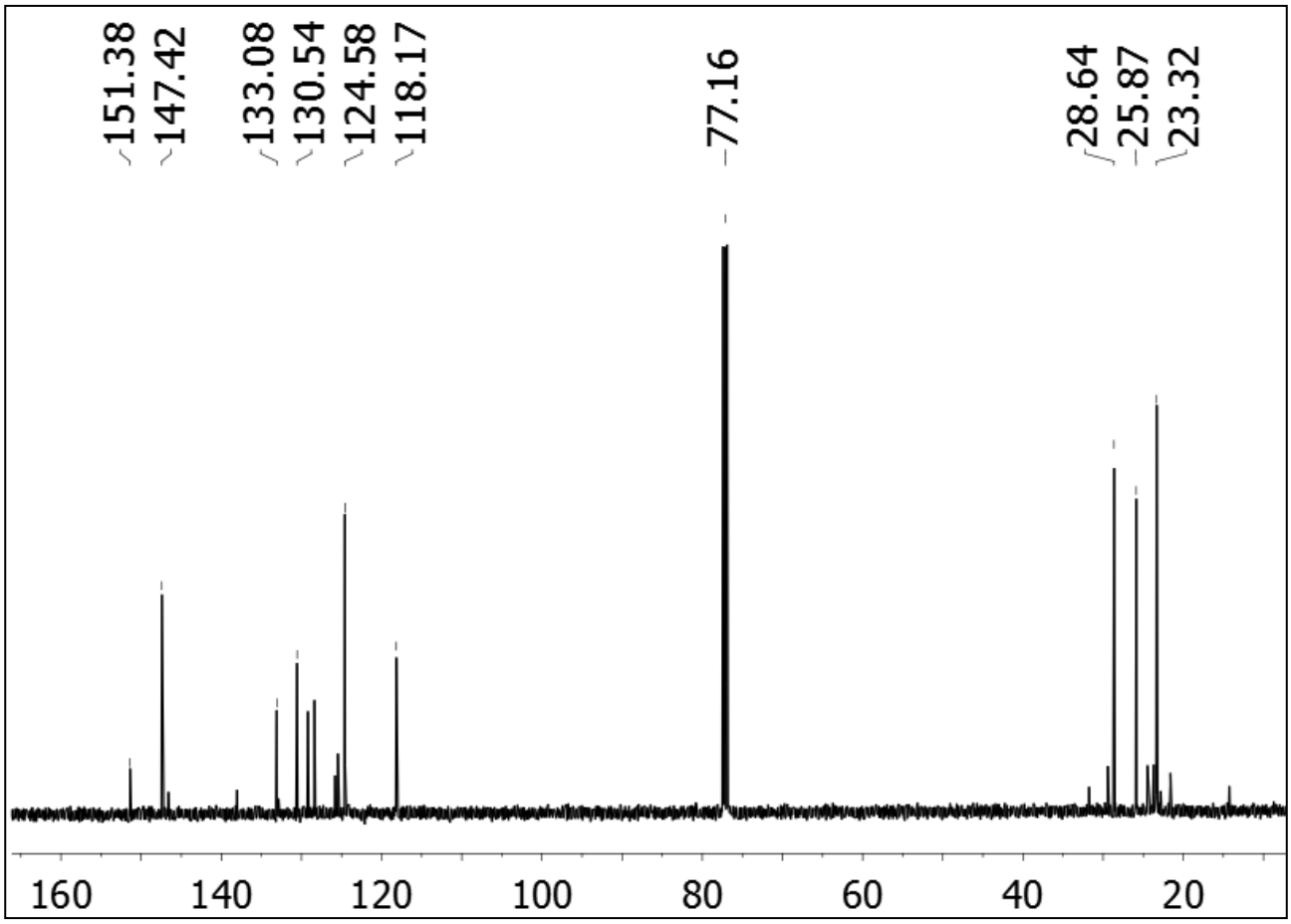


**Fig. S8** $^{13}C\{^{1}H\}$ NMR spectrum (125.8 MHz, $CDCl_3$) of crude **6** as obtained *via* conversion of $\{LLi\}_2$ (**8**) with 2 eq $AlCl_3$ in toluene (*cf.* Experimental section in main article).

**Procedure for the synthesis of {$\mu$-LLi}$_2$ (8)**

**Synthesis of {$\mu$-LLi}$_2$ (8)** In a Schlenk tube equipped with a rubber septum and a magnetic stirrer bar a suspension of LH (5.13 g, 12.7 mmol) in toluene (50 mL) was cooled to 0 °C. Under stirring, a solution (1.6 M) of n-butyllithium in hexane (9.2 mL, 14.7 mmol) was carefully added *via* syringe. The septum was exchanged for a glass stopper and the reaction mixture was stirred over night while warming to room temperature. A pale orange solution formed which was left for another 12 h at room temperature and then kept at 4 °C over night. The Schlenk vessel was placed in the freezer (−30 °C) and stored for 5 d. The pale orange crystal fraction which was obtained by this method contained single crystals suitable for X-ray structure analysis (*cf.* Table S2). The supernatant was removed and the solid dried *in vacuo* for 3 h. The concomitant loss of crystalline appearance is associated with the liberation of toluene from the lattice (*cf.* the molecular structure of **8**, Fig. S3). Yield: 3.62 g, 69%.

$^1$H NMR (500.1 MHz, $C_6D_6$): $\delta$ = 7.15 (m, 4 H, DippH-4), 7.08 (m, 8 H, DippH-3,5), 6.07 (s, 4 H, NC*H*), 3.25 (sept, $J$ = 7, 8 H, C*H*($CH_3$)$_2$), 1.19 (d, $J$ = 7, 24 H, CH(C*H*$_3$)$_2$), 1.11 (d, $J$ = 7, 24 H, CH(C*H*$_3$)$_2$); $^{13}$C{$^1$H} NMR (125.8 MHz, $C_6D_6$): $\delta$ = 149.2 (N*C*N), 141.6 (DippC-1), 137.7 (DippC-2,6), 128.4 (DippC-4), 123.8 (DippC-3,5), 111.1 (N*C*H), 28.6 (*C*H($CH_3$)$_2$), 24.2 (CH(*C*H$_3$)$_2$), 24.0 (CH(*C*H$_3$)$_2$).

**Details of the quantum-mechanical calculations**

DFT calculations of model compounds **2'**, **II'**, **V'**, and **VI'** were carried out at B3LYP/6-31G(d) level of theory with the GAUSSIAN 03 program. The NBO approach was used to calculate the orbital populations, Wiberg Bond Indices (WBI), and Natural Population Analysis (NPA). Cartesian coordinates of optimized structures are shown in Table S3-S6, respectively. The structures obtained by the reported X-ray analyses were used as the input for these calculations.

**Table S3** Cartesian geometry of **2'** in Angstrom [Å].

| Atom type | X coordinates | Y coordinates | Z coordinates |
|---|---|---|---|
| Al | 1.415199 | 0.004824 | 0.010682 |
| Al | -1.416861 | -0.004740 | 0.010618 |
| N | -0.004731 | 1.323141 | 0.007120 |
| N | 1.047205 | 3.487175 | -0.287641 |
| N | -1.084195 | 3.479127 | 0.249342 |
| N | 0.002826 | -1.323095 | 0.013244 |
| N | 1.089888 | -3.475956 | 0.243416 |
| N | -1.041604 | -3.489693 | -0.293228 |
| C | -0.012470 | 2.616349 | -0.007904 |
| C | 0.622593 | 4.818576 | -0.206902 |
| C | -0.679660 | 4.813759 | 0.129703 |
| C | 2.363644 | 3.124380 | -0.716585 |
| C | 3.334055 | 2.767817 | 0.222418 |
| C | 4.628777 | 2.470744 | -0.206235 |
| C | 4.953737 | 2.543567 | -1.560892 |
| C | 3.981923 | 2.910057 | -2.495085 |
| C | 2.685305 | 3.199283 | -2.075457 |
| C | -2.391735 | 3.108779 | 0.699837 |
| C | -2.690927 | 3.178959 | 2.064008 |
| C | -3.978782 | 2.881801 | 2.504597 |
| C | -4.964269 | 2.513325 | 1.585689 |
| C | -4.661764 | 2.445372 | 0.225544 |
| C | -3.375562 | 2.748972 | -0.223699 |
| C | 0.014486 | -2.616158 | -0.008221 |
| C | 0.691486 | -4.811484 | 0.113975 |
| C | -0.610800 | -4.819736 | -0.222427 |
| C | 2.393266 | -3.102662 | 0.704040 |
| C | 2.678210 | -3.159763 | 2.071831 |

| | | | |
|---|---|---|---|
| C | 3.961688 | -2.859252 | 2.522818 |
| C | 4.957082 | -2.501245 | 1.610518 |
| C | 4.668845 | -2.446509 | 0.246659 |
| C | 3.386814 | -2.752562 | -0.212734 |
| C | -2.361889 | -3.130375 | -0.712423 |
| C | -2.696047 | -3.215356 | -2.067715 |
| C | -3.996632 | -2.929908 | -2.477494 |
| C | -4.959953 | -2.556504 | -1.537238 |
| C | -4.622506 | -2.473508 | -0.186239 |
| C | -3.323937 | -2.767495 | 0.232799 |
| H | 2.253580 | 0.097591 | 1.376881 |
| H | 2.255223 | -0.084977 | -1.354832 |
| H | -2.255730 | -0.089627 | 1.377063 |
| H | -2.256669 | 0.076877 | -1.355567 |
| H | 1.305548 | 5.631315 | -0.395083 |
| H | -1.374219 | 5.621390 | 0.296129 |
| H | 3.069616 | 2.715111 | 1.272652 |
| H | 5.380842 | 2.182429 | 0.522440 |
| H | 5.963467 | 2.313838 | -1.890457 |
| H | 4.231073 | 2.962079 | -3.551246 |
| H | 1.914973 | 3.473578 | -2.789845 |
| H | -1.910288 | 3.456247 | 2.765912 |
| H | -4.210528 | 2.929873 | 3.564884 |
| H | -5.967304 | 2.278034 | 1.931407 |
| H | -5.424628 | 2.155139 | -0.491062 |
| H | -3.127202 | 2.698013 | -1.277986 |
| H | 1.389578 | -5.617196 | 0.274846 |
| H | -1.290237 | -5.634161 | -0.415972 |
| H | 1.890163 | -3.429765 | 2.768254 |
| H | 4.182398 | -2.896933 | 3.585867 |
| H | 5.956783 | -2.263673 | 1.964255 |
| H | 5.439526 | -2.164309 | -0.464786 |
| H | 3.148729 | -2.710628 | -1.269798 |
| H | -1.932135 | -3.494221 | -2.787225 |
| H | -4.255452 | -2.989977 | -3.530909 |
| H | -5.972728 | -2.329460 | -1.859222 |
| H | -5.367835 | -2.179920 | 0.547227 |

| | | | |
|---|---|---|---|
| H | -3.050540 | -2.707986 | 1.280383 |

**Table S4** Cartesian geometry of **II'** in Angstrom [Å].

| Atom type | X coordinates | Y coordinates | Z coordinates |
|---|---|---|---|
| Al | 0.000008 | -0.996466 | -0.000264 |
| N | 1.432244 | 0.315061 | -0.000173 |
| N | -1.432246 | 0.315062 | -0.000085 |
| C | 2.478741 | 2.544465 | -0.000144 |
| C | 1.262988 | 1.641537 | -0.000147 |
| C | -0.000001 | 2.259488 | -0.000162 |
| C | -1.262991 | 1.641534 | -0.000072 |
| C | -2.478744 | 2.544464 | 0.000009 |
| C | 2.754559 | -0.246113 | -0.000021 |
| C | 3.388675 | -0.554757 | 1.210448 |
| C | 4.654518 | -1.142062 | 1.207407 |
| C | 5.292039 | -1.434060 | 0.000214 |
| C | 4.654375 | -1.142862 | -1.207091 |
| C | 3.388529 | -0.555553 | -1.210358 |
| C | -2.754560 | -0.246115 | 0.000036 |
| C | -3.388710 | -0.555114 | -1.210321 |
| C | -4.654555 | -1.142422 | -1.207080 |
| C | -5.292039 | -1.434061 | 0.000215 |
| C | -4.654340 | -1.142504 | 1.207418 |
| C | -3.388496 | -0.555197 | 1.210485 |
| H | 0.000126 | -1.824764 | 1.368284 |
| H | -0.000129 | -1.824442 | -1.368996 |
| H | 3.105112 | 2.354853 | -0.878433 |
| H | 3.104993 | 2.355073 | 0.878269 |
| H | 2.185160 | 3.595804 | -0.000295 |
| H | -0.000002 | 3.341996 | -0.000178 |
| H | -2.185162 | 3.595803 | 0.000102 |
| H | -3.105074 | 2.354880 | 0.878326 |
| H | -3.105037 | 2.355044 | -0.878376 |
| H | 2.879710 | -0.336511 | 2.144794 |
| H | 5.139638 | -1.376259 | 2.151206 |
| H | 6.276294 | -1.894176 | 0.000314 |
| H | 5.139380 | -1.377670 | -2.150796 |

| | | | |
|---|---|---|---|
| H | 2.879457 | -0.337910 | -2.144785 |
| H | -2.879770 | -0.337144 | -2.144745 |
| H | -5.139699 | -1.376890 | -2.150798 |
| H | -6.276295 | -1.894176 | 0.000292 |
| H | -5.139320 | -1.377040 | 2.151204 |
| H | -2.879396 | -0.337280 | 2.144834 |

**Table S5** Cartesian geometry of **V'** in Angstrom [Å].

| Atom type | X coordinates | Y coordinates | Z coordinates |
|---|---|---|---|
| C | 3.691139 | -1.458086 | -0.744385 |
| Al | 0.000067 | -1.395005 | -0.000604 |
| P | 2.846716 | -0.000017 | -0.028736 |
| C | 3.323568 | -0.001434 | 1.744352 |
| N | 1.285500 | 0.000033 | -0.310060 |
| C | -3.690433 | -1.458294 | 0.745019 |
| C | 3.690709 | 1.459424 | -0.742053 |
| C | -3.325114 | -0.001087 | -1.743728 |
| N | -1.285291 | 0.000095 | 0.308771 |
| P | -2.846747 | -0.000005 | 0.028953 |
| Al | 0.000125 | 1.395134 | -0.000569 |
| C | -3.690282 | 1.459227 | 0.743254 |
| H | 3.509188 | -1.485771 | -1.822637 |
| H | 3.275804 | -2.368233 | -0.300022 |
| H | 4.769506 | -1.429530 | -0.556667 |
| H | -0.409278 | -2.284441 | -1.286432 |
| H | 0.409334 | -2.284385 | 1.285331 |
| H | 2.895052 | 0.884870 | 2.222287 |
| H | 4.410513 | -0.001907 | 1.880343 |
| H | 2.894448 | -0.888163 | 2.220945 |
| H | -3.507895 | -1.486040 | 1.823171 |
| H | -3.275115 | -2.368299 | 0.300347 |
| H | -4.768910 | -1.429992 | 0.557895 |
| H | 3.509196 | 1.488536 | -1.820344 |
| H | 4.769016 | 1.431175 | -0.553960 |
| H | 3.274700 | 2.368713 | -0.296569 |
| H | -2.896707 | 0.885153 | -2.221885 |

| | | | |
|---|---|---|---|
| H | -4.412172 | -0.001178 | -1.878826 |
| H | -2.896675 | -0.887873 | -2.220834 |
| H | -0.409128 | 2.284618 | -1.286392 |
| H | 0.409499 | 2.284309 | 1.285470 |
| H | -3.274942 | 2.368658 | 0.297433 |
| H | -3.507671 | 1.488273 | 1.821360 |
| H | -4.768773 | 1.430748 | 0.556243 |

**Table S6** Cartesian geometry of **VI'** in Angstrom [Å].

| Atom type | X coordinates | Y coordinates | Z coordinates |
|---|---|---|---|
| C | 3.252117 | -0.000096 | -0.000089 |
| C | 2.617067 | 1.240048 | -0.001069 |
| C | 1.262471 | 1.556414 | -0.000870 |
| C | 0.102073 | 0.744993 | -0.000024 |
| C | 0.102022 | -0.744993 | 0.000119 |
| C | 1.262380 | -1.556482 | 0.001207 |
| C | 2.616999 | -1.240188 | 0.001090 |
| N | -1.127754 | 1.275182 | 0.000337 |
| Al | -2.568054 | 0.000030 | 0.000201 |
| N | -1.127796 | -1.275085 | -0.000477 |
| C | -1.327722 | -2.716520 | -0.001197 |
| C | -1.327475 | 2.716629 | 0.000647 |
| H | 4.338673 | -0.000125 | -0.000244 |
| H | 3.278128 | 2.105473 | -0.002031 |
| H | 1.060265 | 2.621543 | -0.001731 |
| H | 1.060100 | -2.621599 | 0.002370 |
| H | 3.278000 | -2.105660 | 0.002038 |
| H | -3.413607 | 0.000251 | -1.360652 |
| H | -3.412538 | -0.000206 | 1.361748 |
| H | -0.892010 | -3.192245 | -0.890652 |
| H | -0.895066 | -3.192799 | 0.889479 |
| H | -2.400899 | -2.925236 | -0.003065 |
| H | -2.400619 | 2.925537 | 0.001864 |
| H | -0.892229 | 3.192524 | 0.890250 |
| H | -0.894237 | 3.192653 | -0.889883 |