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Supporting Information for

Synthesis of Novel Chiral Heterometallic Terpene Oximates: Unusual Generation of an Aluminium Enolate by a Cooperative Effect

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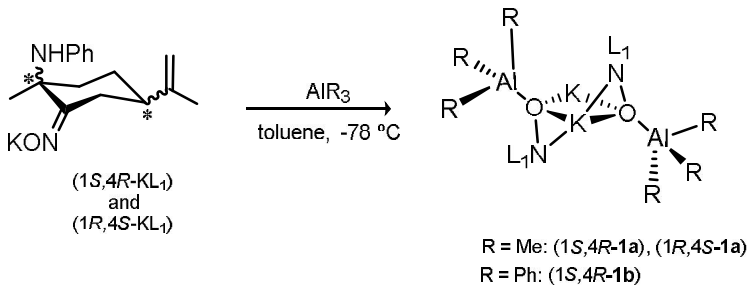
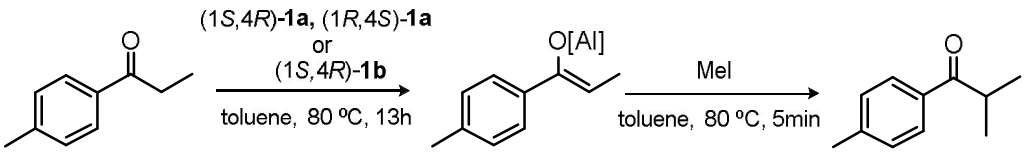


Scheme S1. Synthesis of compounds **1a** and **(*1S, 4R*)-1b**



Scheme S2. Alkylation of *p*-methylpropiophenone.

CONTENS

I. Experimental details and physical data

General Considerations. All manipulations were conducted using Schlenk techniques in conjunction to an inert atmosphere glove box. All solvents were rigorously dried prior to use. NMR spectra were recorded at 400.13 (^{1}H), 100.62 (^{13}C), 40.50 (^{15}N) and MHz on a Bruker AV400. Chemical shifts (δ) are given in ppm using C_6D_6 as solvent. ^{1}H and ^{13}C resonances were measured relative to solvent peaks considering TMS δ = 0 ppm. Elemental analyses were obtained on a Perkin-Elmer Series II 2400 CHNS/O analyzer.

1. Synthesis of (1*S*,4*R*)-HONL$_1$. Ligand was prepared as previously described in the literature.[1].

Synthesis of (1*R*,4*S*)-HONL$_1$. To a mixture of *S*-limonene 6.0 g (44 mmol) and isopentylnitrite 6 mL (44 mmol), 9 mL of HCl (37%, 92.5 mmol) was added dropwise for 90 min to -5 ºC. The solid was filtered and washed with cold methanol. Yield: 68% (6 g, 14.96 mmol).To a suspension of this solid in 10 mL of ethanol was added 6 mL of aniline (59.85 mmol) to 70 ºC. When the mixture was dissolved, 15 mL of HCl was added dropwise at -5 ºC. The solid was filtered and washed with ethanol and diethyl ether. Yield: 53 %. (4.64 g, 15.75 mmol). To a suspension of this solid in 15 ml of diethyl ether was added 4mL of triethylamine. The mixture was stirred for 12 hours, and then was filtered. The solvent was removed under vacuum and a yellow oil was obtained. This oil was precipitated and washed with hexane.

^{1}H-NMR (400.13 MHz,298 K, C_6D_6): δ 9.17 (s, 1H, OH), 7.09 (m, 2H, *m*-C_6H_5-*H*), 6.76 (m, 2H, *o*-C_6H_5-*H*), 6.72 (m, 1H, *p*-C_6H_5-*H*), 4.70 (s, 2H, =CH_2), 3.60 (m, 1H,-CH_2^3), 3.10 (s, 1H, N*H*), 2.08, (m, 1H,-CH_2^3), 2.05 (m, 1H,-CH^4),1.56 (m, 1H,-CH_2^5), 1.55 (s, 3H, CH_3-C=), 1.53 (s, 3H, CH_3-C^1), 1.38 (m, 1H, CH_2^6), 1.37 (m, 1H,-CH_2^5), 1.29 (m, 1H, CH_2^6).

^{13}C-NMR (100.62 MHz, 298 K, C_6D_6): δ 164.6 (-*C*^{2}) 148.2 (-*C*=CH_2), 146.8 (C_{ipso}), 129.5, 118.8, 115.5, (-C_6H_5), 109.8 (*C*H_2=), 56.9(*C*^{1}), 45.9 (*C*H^4), 43.1 (*C*H_2^6), 26.6 (*C*H_2^5), 26.3 (*C*H_2^3), 23.2 (*C*H$_3$-C^1), 20.6 (*CH*$_3$-C=).

E.A. (%) $C_{16}H_{22}N_2O$ (258.17): *calcd:* C = 74.38, N = 10.84, H = 8.58. *found:* C = 74.56, N = 10.84, H = 8.13.

2. Synthesis of (1*S*,4*R*)-KONL$_1$ and (1*R*,4*S*)-KONL$_1$. To a solution of 0.30 g (1.15 mmol) of (1*S*,4*R*) and (1*R*,4*S*) -1-phenylamino-4-isopropenyl-1-methyl-6-cyclohexanoxime (**(1*S*,4*R*) and (1*R*,4*S*) -HONL$_1$**) in 20 mL of toluene, 0.15 g (1.15 mmol) of KBn were added, in a cold bath of dry ice/isopropanol, and the mixture was stirred for 30 min. The solvent was removed under vacuum and a yellow solid was isolated, which was washed with hexane. Yield: 90%

^{1}H-RMN (400.13 MHz,298 K, C_6D_6): δ 7.13 (m, 2H, *m*-C_6H_5-*H*), 6.76 (m, 2H, *o*-C_6H_5-*H*), 6.71 (m, 1H, *p*-C_6H_5-*H*), 4.91 (br, 1H, =CH_2), 4.82 (br, 1H, =CH_2), 3.70 (m, 1H,-CH_2^3), 3.37 (s, 1H, N*H*), 2.24, (m, 1H,-CH^4), 1.99 (m, 1H,-CH_2^3), 1.72 (s, 3H, CH_3-C=),1.62 (m, 1H, CH_2^5), 1.59 (m, 2H, CH_2^6), 1.51 (m, 1H, CH_2^5), 1.51 (s, 3H, CH_3-C^1).

^{13}C-NMR (100.62 MHz, 298 K, C_6D_6): δ 157.4 (-*C*^{2}) 149.5 (-*C*=CH$_2$), 147.7(*C*$_{ipso}$), 129.1, 118.4, 116.0, (-*C*$_6$H$_5$), 109.5 (*C*H$_2$=), 57.3 (*C*^{1}), 45.5 (*C*H^4), 42.2 (*C*H$_2^6$), 27.1 (*C*H$_2^3$), 25.5 (*C*H$_2^5$), 24.9(*C*H$_3$-C^1), 20.9 (*C*H$_3$-C=).

A.E. (%) $C_{16}H_{21}ON_2K\cdot 1/4\ C_7H_8$ (296.13): *calcd*: C = 66.73, N = 8.77, H = 7.26. *found*: C = 66.63, N = 9.10, H = 7.62.

3. Synthesis of [AlMe$_3$K(tol)(ONL$_1$)]$_2$ ((*1S, 4R*) and (*1R, 4S*)-1a). To a solution of 0.344 g (1.15 mmol) of (**(*1S, 4R*) and (*1R, 4S*) -KONL$_1$**) in 20 mL of toluene, 0.58 mL of AlMe$_3$ (2M in toluene, 1.15 mmol) were added in a cold bath of dry ice/isopropanol. The solution was stirred for 30 min, filtered and conserved to -5 ºC. After one day colorless crystals of compound **(*1S, 4R*)-1a** were observed. Yield: 97% (0.417 g, 0.56 mmol).

^{1}H-NMR (400.13 MHz,298 K, C_6D_6): δ 7.31 (m, 2H, *m*-C_6H_5-*H*), 6.83 (m, 1H, *p*-C_6H_5-*H*), 6.81 (m, 2H, *o*-C_6H_5-*H*), [Tol: 7.13 (m, 2H, *m*-C_6H_5-*H*), 7.05 (*p*-C_6H_5-*H*), 7.01 (m, 2H, *o*-C_6H_5-*H*), 2.11 (s, 3H, -CH_3)], 4.90 (br, 1H, =CH_2), 4.80 (br, 1H, =CH_2), 3.32 (m, 1H,-CH_2^3), 3.15 (s, 1H, -N*H*), 2.26 (m, 1H, -CH^4), 2.23 (m, 1H, -CH_2^3), 1.69 (s, 3H, CH_3-C=), 1.67 (m, 1H, CH_2^5), 1.57 (m, 2H, CH_2^6), 1.51 (m, 1H, CH_2^5), 1.38 (s, 3H, CH_3-C^1), -0.67 (s, 9H, Al-CH_3).

^{13}C-NMR (100.62 MHz, 298 K, C_6D_6): δ 169.2 (-*C*^{2}) 148.7 (-*C*=CH$_2$), 146.6 (*C*$_{ipso}$), 129.4, 118.8, 115.9, (-*C*$_6$H$_5$), [Tol:137.6(C$_{ipso}$) 129.1, 128.3, 125.4 (-*C*$_6$H$_5$), 21.1 (-*C*H$_3$)], 109.8 (*C*H$_2$=), 57.1 (*C*^{1}), 45.7 (*C*H^4), 42.6 (*C*H$_2^6$), 26.7 (*C*H$_2^3$), 26.5 (*C*H$_2^5$), 23.7 (*C*H$_3$-C^1), 20.3 (*C*H$_3$-C=), -6.6 (Al-*C*H$_3$).

E.A. (%) $C_{38}H_{60}Al_2K_2N_4O_2\cdot$1tol (829,22): *calcd:* C = 65.18, N = 6.76, H = 8.27. *found:* C = 65.37, N= 6.55, H = 8.19.

4. Synthesis of [$AlPh_3K(\{1S,4R\}\text{-}ONL_1)]_x$ ((1*S*,4*R*)-1b). To a solution of 0.344 g (1.15 mmol) of (**(1*S*,4*R*) and (1*R*,4*S*) -$KONL_1$**) in 20 mL of toluene, 1.16 mL of $AlPh_3$ (1M in Bu_2O, 1.15 mmol) were added in a cold bath of dry ice/isopropanol. The solution was stirred for 30 min and conserved to -21 ºC. After one month colorless crystals of compound **1b** were observed. Yield: 82% (0.517 g, 0.471 mmol).

^{1}H-NMR (400.13 MHz, 298 K, C_6D_6): δ 8.07 (m, 6H, *o*-AlC_6H_5-*H*), 7.30 (m, 6H, *m*-AlC_6H_5-*H*), 7.22 (m, 3H, *p*-AlC_6H_5-*H*), 6.95 (m, 2H, *m*-C_6H_5-*H*), 6.63 (m, 1H, *p*-C_6H_5-*H*), 6.48 (m, 2H, *o*-C_6H_5-*H*), 5.09 (br, 1H, =CH_2), 4.92 (br, 1H, =CH_2), 3.03 (s, 1H, -N*H*), 2.98 (m, 1H,-CH_2^3), 2.91 (m, 1H,-CH_2^3), 1.91 (m, 1H, CH^4), 1.77 (m, 1H, CH_2^6), 1.66 (s, 3H, CH_3-C=), 1.60 (m, 1H, CH_2^5), 1.40 (m, 1H, CH_2^5), 1.21 (m, 1H, CH_2^6), 1.19 (s, 3H, CH_3-C^1).

^{13}C-NMR (100.62 MHz, 298 K, C_6D_6): δ 163.8(-C^2), 155.0(C_{ipso}-AlC_6H_5) 148.2(C_{ipso}-C_6H_5), 146.0 (-*C*=CH_2), 138.6 (*o*-AlC_6H_5), 129.5 (*m*-C_6H_5), 127.5 (*m*-AlC_6H_5), 127.3 (*p*-AlC_6H_5), 119.6 (*o*-C_6H_5), 117.7 (*p*-C_6H_5), 110.8 (CH_2=), 58.2 (C^1), 42.6 (CH^4), 37.16 (CH_2^6), 26.3 (CH_3-C^1), 26.0 (CH_2^3), 25.6 (CH_2^5), 21.6 (CH_3-C=).

E.A. (%) $C_{67}H_{71}Al_2K_2N_4O_2$ (1108.46): *calcd:* C = 73.61, N = 5.05, H = 6.54. *found:* C = 72.71, N = 5.30, H = 6.72

5. Synthesis of (2). To a Schlenk containing 0.65g of crystals of compound **1a** (0.88 mmol) in toluene, 250 μL of *p*-methylpropiophenone (1.76 mmol) was added, and the mixture was stirred for 13 h at 80 ºC. The solvent was then removed under vacuum to give a yellow oil which was characterized as **2**.

^{1}H-NMR (400.13 MHz, 298 K, C_6D_6): δ 7.73 (m, 1H, *o*-C_6H_4-*H*) 7.25 (m, 2H, *m*-C_6H_5-*H*), 6.89 (m, 1H, *m*-C_6H_4-*H*) 6.83 (m, 2H, *o*-C_6H_5-*H*), 6.78 (m, 1H, *p*-C_6H_5-*H*), 5.26 (m, 0.5H, *H*C=CO-), 4.88 (br, 1H, =CH_2), 4.76 (br, 1H, =CH_2), 3.42 (m, 1H,-CH_2^3), 3.25 (s, 1H, -N*H*), 2.31 (m, 1H,-CH_2^3), 2.31 (m, 1H, CH^4), 2.00 (s, 1.5H, *p*-CH_3-C_6H_4-), 1.98 (s, 1.5H, CH_3-CH=CO-), 1.72 (m, 1H, CH_2^5), 1.71 (m, 2H, CH_2^6), 1.65 (s, 3H, CH_3-C=), 1.53 (s, 3H, CH_3-C^1), 1.51 (m, 1H, CH_2^5), -0.49 (br, 7.5H, Al(CH_3)$_{2.5}$).

^{13}C-NMR (100.62 MHz, 298 K, C_6D_6): δ 201.2 (-*C*=O), 169.6 (-C^2) 153.4 (*C*-OAl(CH_3)$_2$) 148.9 (-*C*=CH_2), 146.9 (-NH-C_{ipso}), 143.46 (-C_{ipso}-C-OAl), 140.0 (-C_{ipso}-C=O), 137.9 (Me-C_{ipso}-enolate), 129.3 (*m*-C_6H_4), 129.3 (*m*-C_6H_5), 125.7 (*o*-C_6H_4), 116.4 (*o*-C_6H_5), 116.3 (*p*-C_6H_5), 110.2 (CH_2=), 98.0 (H*C*=CO-), 57.8 (C^1), 45.9 (CH^4),

42.36 (CH_2^6), 27.0 (CH_2^5), 26.8 (CH_2^3), 24.2 (CH_3-C^1), 21.4 (*p*-CH_3), 20.4 (CH_3-C=), 12.5 (CH_3-enolate), -8.4 (Al(CH_3)$_3$) -8.7 (Al(CH_3)$_2$).

E.A. (%) $C_{47}H_{68}Al_2K_2N_4O_3$ (868.42): *calcd:* C = 64.94, N = 6.45, H = 7.89. *found:* C = 65.05, N = 6.31, H = 7.35

6. Synthesis of (3). To a NMR tube containing 0.02g of compound **1b** (0.036 mmol) in toluene, 10.70 μL of *p*-methylpropiophenone (0.072 mmol) was added, and the mixture was heated for 3 h at 80 ºC. The solution was conserved at RT. After one day colorless crystals of compound **3** were observed. Yield: 89% (0.017 g, 0.038 mmol).

7. Synthesis of 2-methyl-1-(4-methylphenyl)-1-propanone (4). To a solution of aluminum enolate **2** or **3**, MeI was added at 90 ºC for 10 min. The solution was filtered and the product was purified by chromatography using a hexane-dichloromethane mixture as eluent.

^{1}H NMR (400.13 MHz, 298 K, $CDCl_3$) δ (ppm): 7.87 (d, 2H, *o*-C_6H_4-*H*), 7.27 (d, 2H, *m*-C_6H_4-*H*), 3.39 (sex, 1H, $^{\alpha}$C*H*), 2.42 (s, 3H, *p*-CH_3), 1.83 (sep, 1H, $^{\beta}$CH_2), 1.49 (sep, 1H, $^{\beta}$CH_2), 1.19 (d, 3H, $^{\beta}$CH_3), 0.92 (s, 3H, $^{\gamma}$CH_3).

II. NMR Spectra

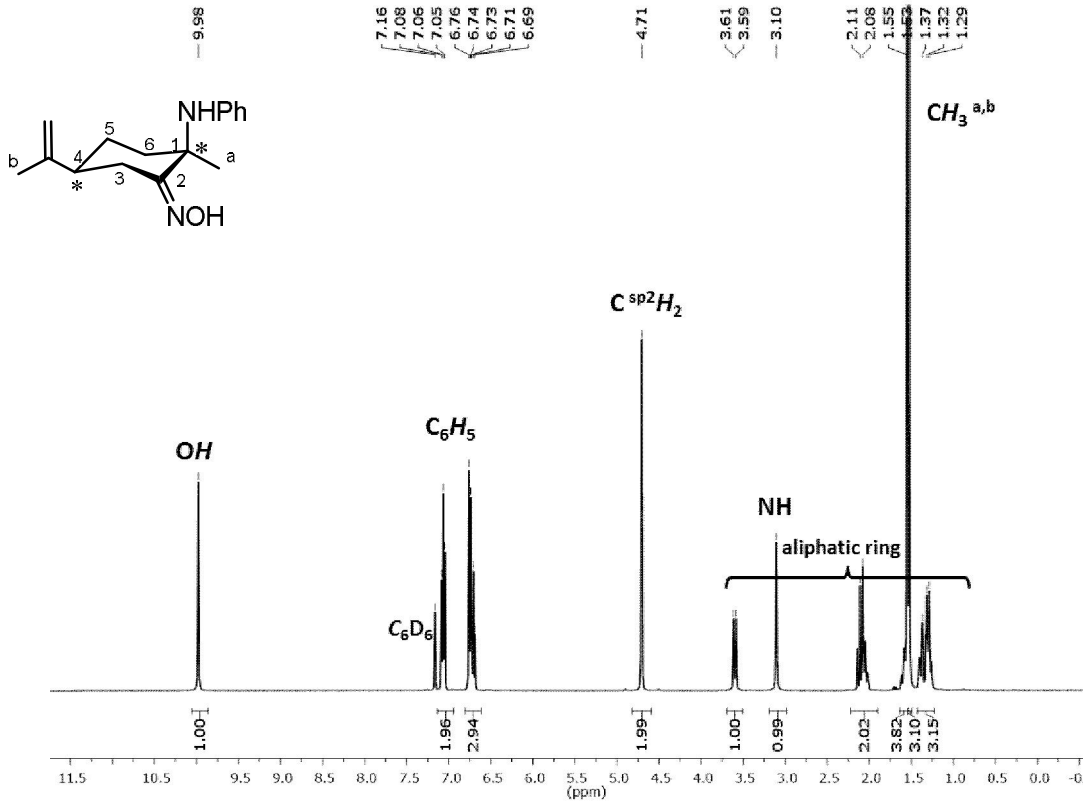


Figure S1. ^{1}H NMR (298K, C_6D_6, 400.13 MHz) spectrum for crystals of **(1*R*,4*S*)-HONL$_1$**.

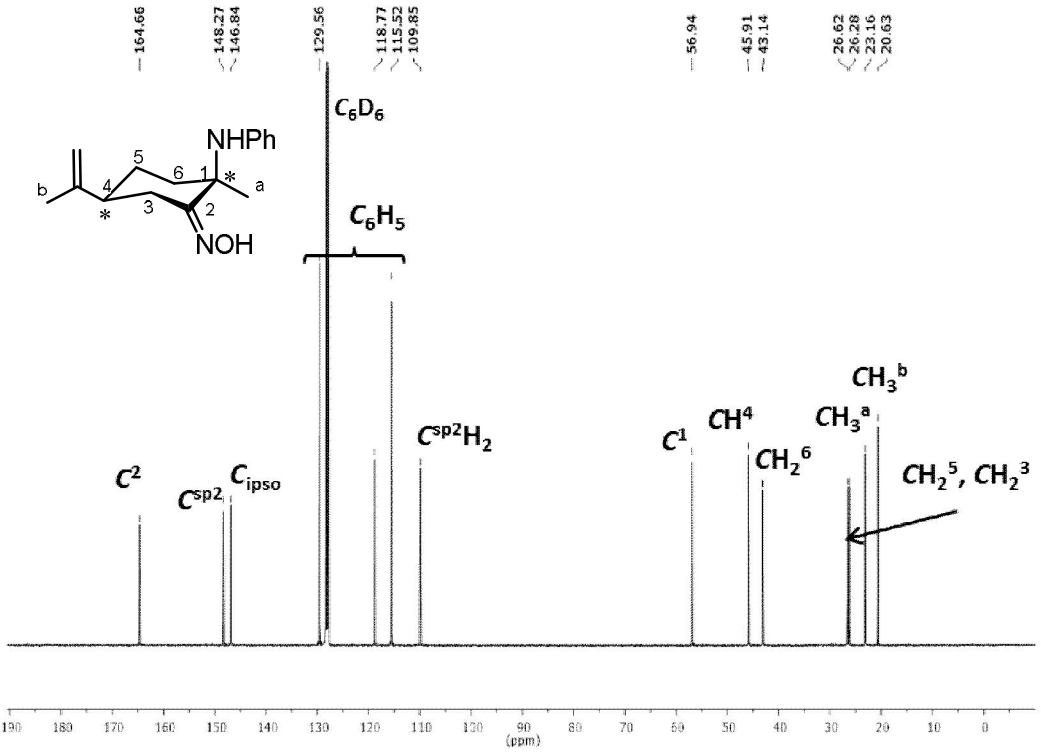


Figure S2. ^{13}C NMR (298K, C_6D_6, 100.62 MHz) spectrum for crystals of **(1*R*,4*S*)-HONL$_1$**.

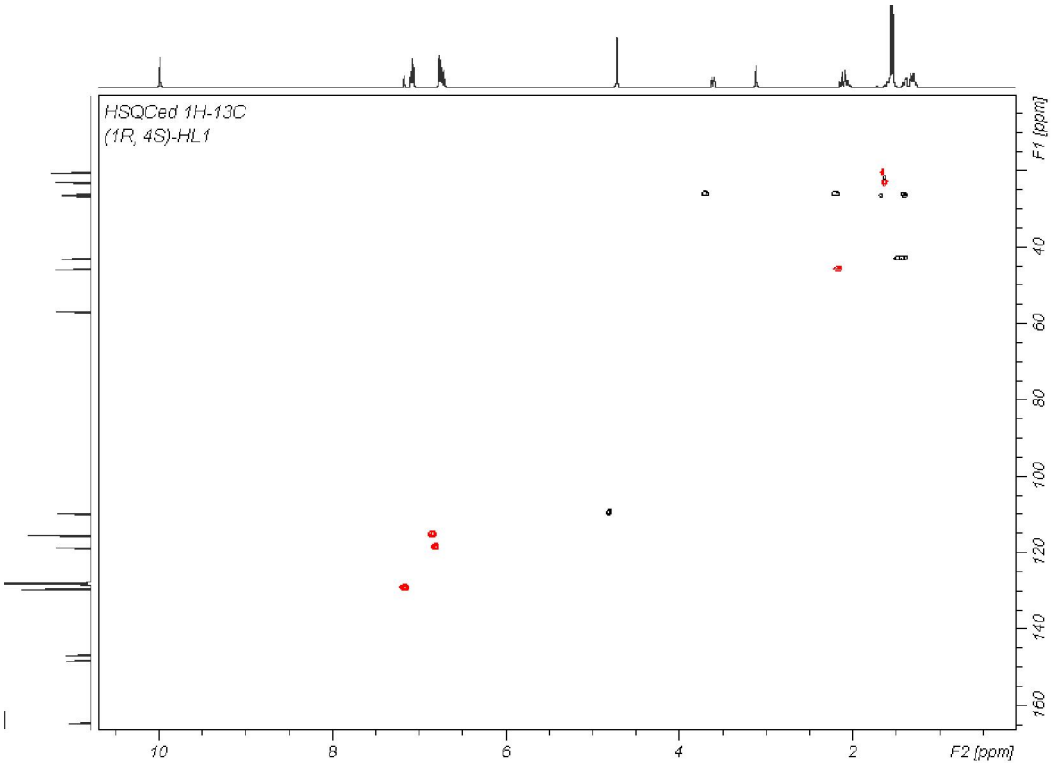


Figure S3. ^{1}H ^{13}C HSQC-*ed* NMR (298K, C_6D_6) spectrum for crystals of **(1*R*,4*S*)-HONL$_1$**. **Note:** Red signals correspond to CH and CH_3 groups. Black signals correspond to CH_2 groups

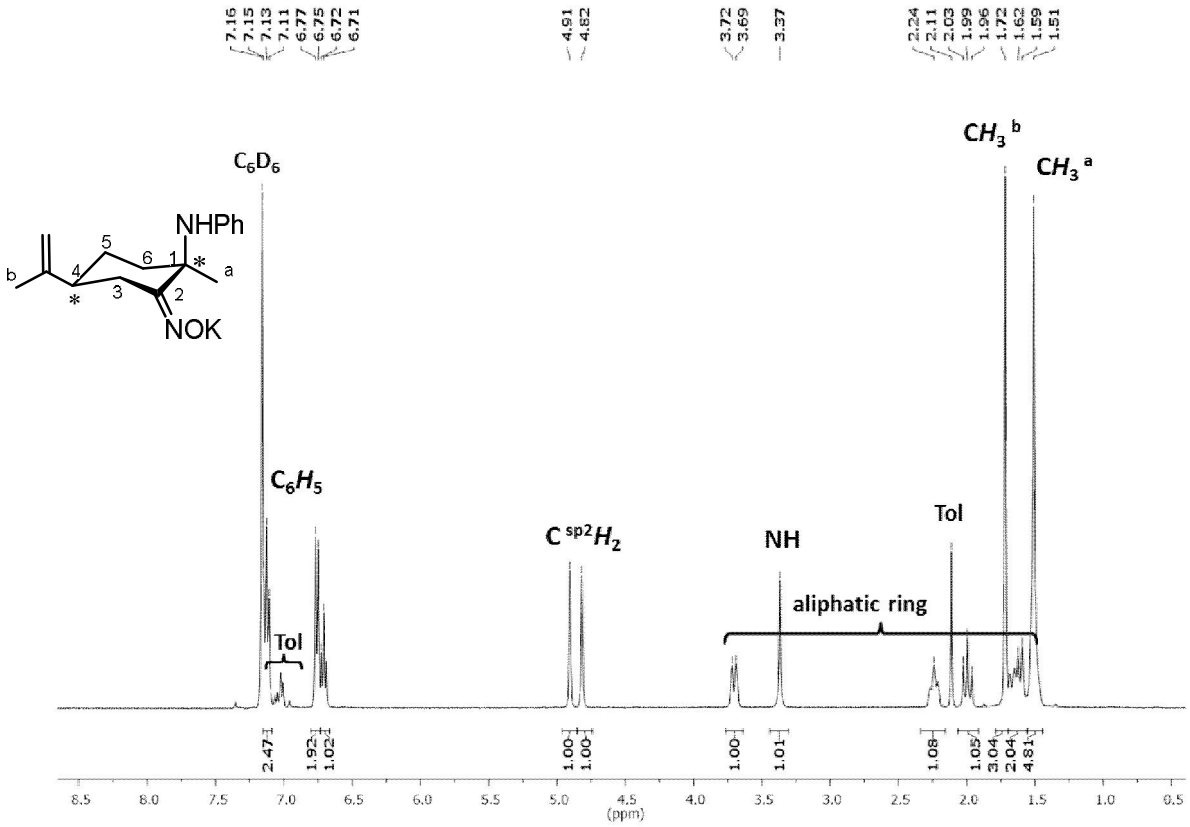


Figure S4. ^{1}H NMR (298K, C_6D_6, 400.13 MHz) spectrum of **(1*S*,4*R*)-KONL$_1$**.

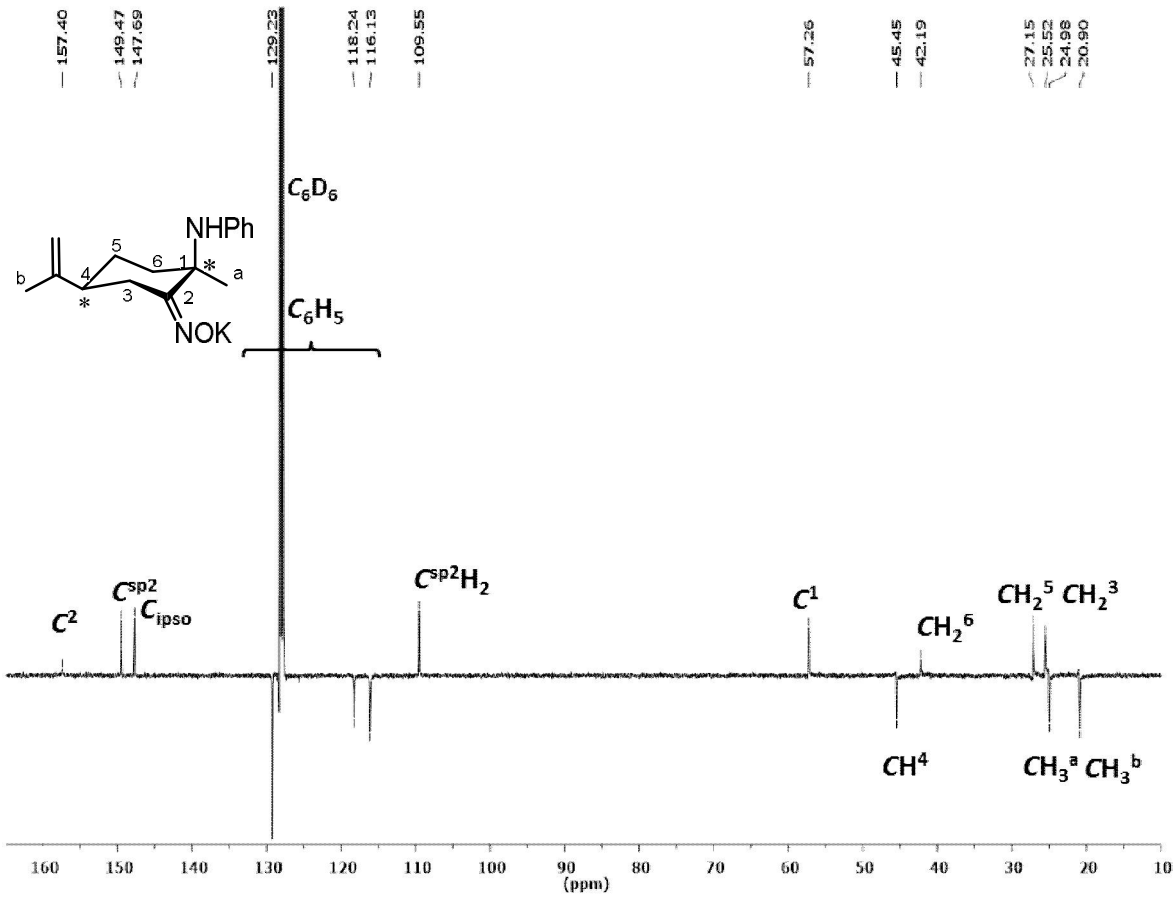


Figure S5. ^{13}C NMR (298K, C_6D_6, 100.62 MHz) spectrum for crystals of **(1*S*,4*R*)-KONL$_1$**.

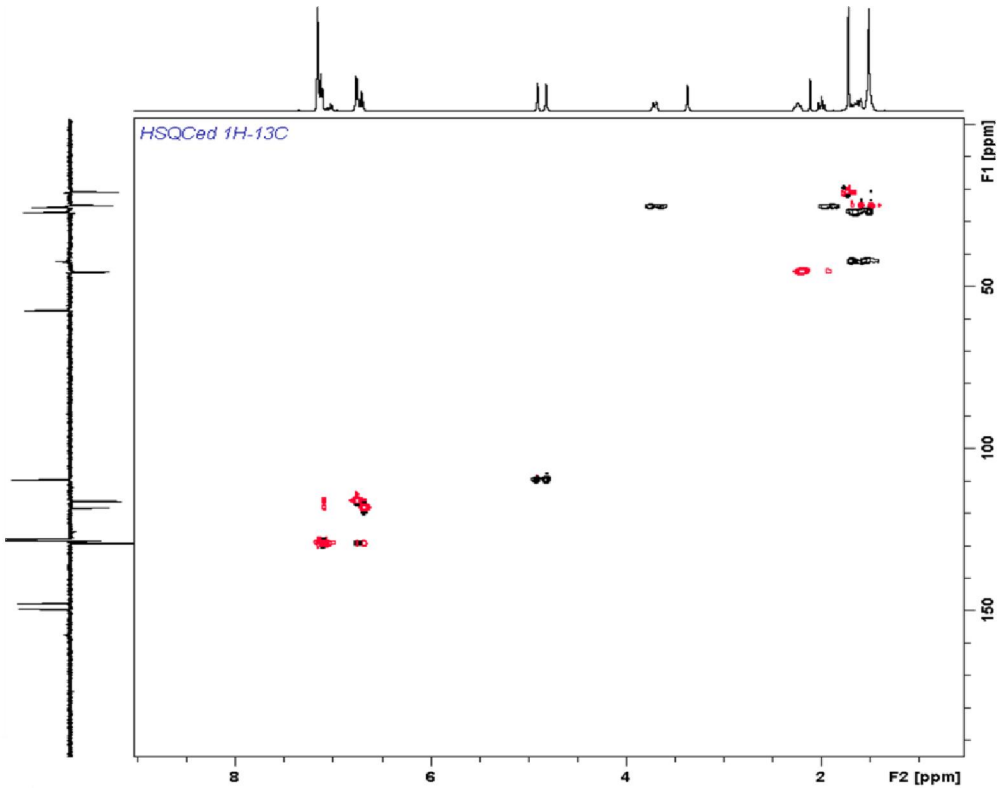


Figure S6. ^{1}H-^{13}C HSQC-*ed* NMR (298K, C_6D_6) spectrum of **(1*S*,4*R*)-KONL$_1$**. **Note:** Red signals correspond to CH and CH_3 groups. Black signals correspond to CH_2 groups.

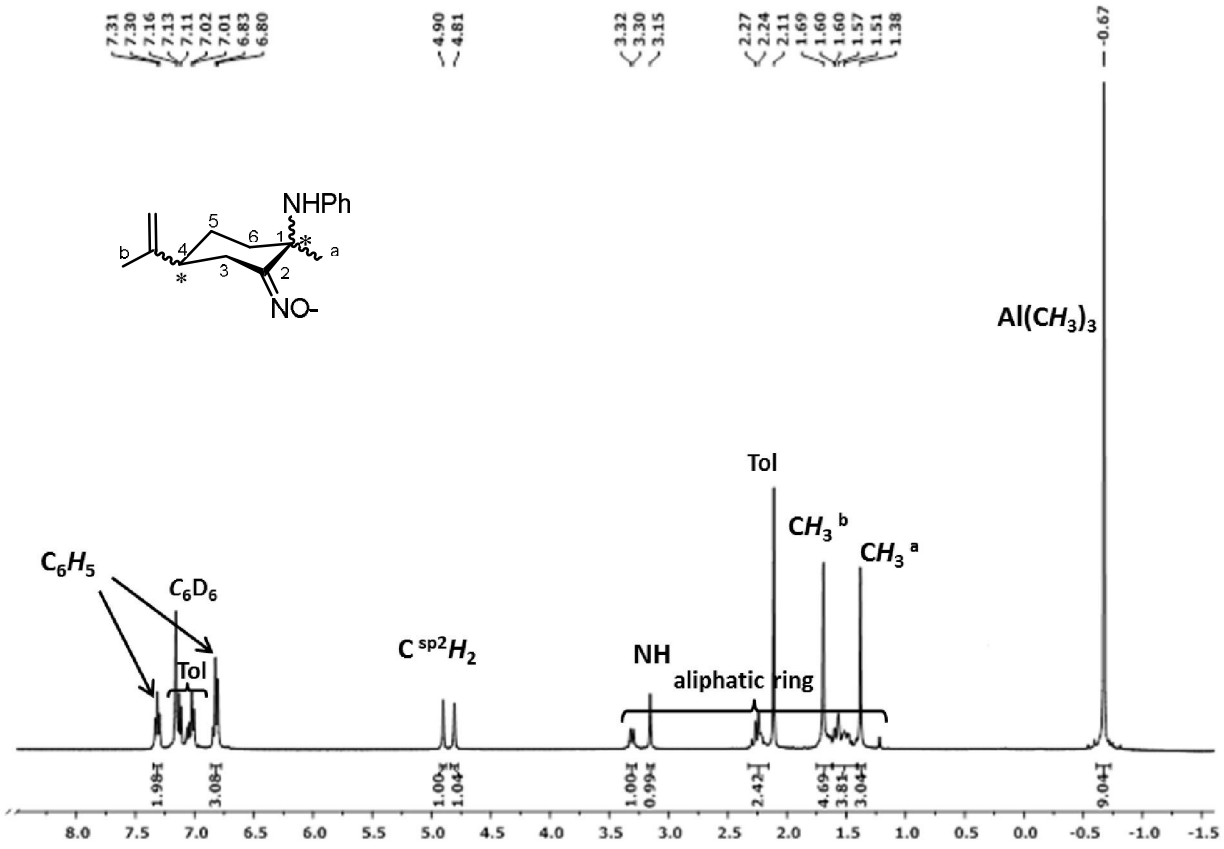


Figure S7. ^{1}H NMR (298K, C_6D_6, 400.13 MHz) spectrum for crystals of **(1*S*,4*R*)-1a** and **(1*R*,4*S*)-1a.**

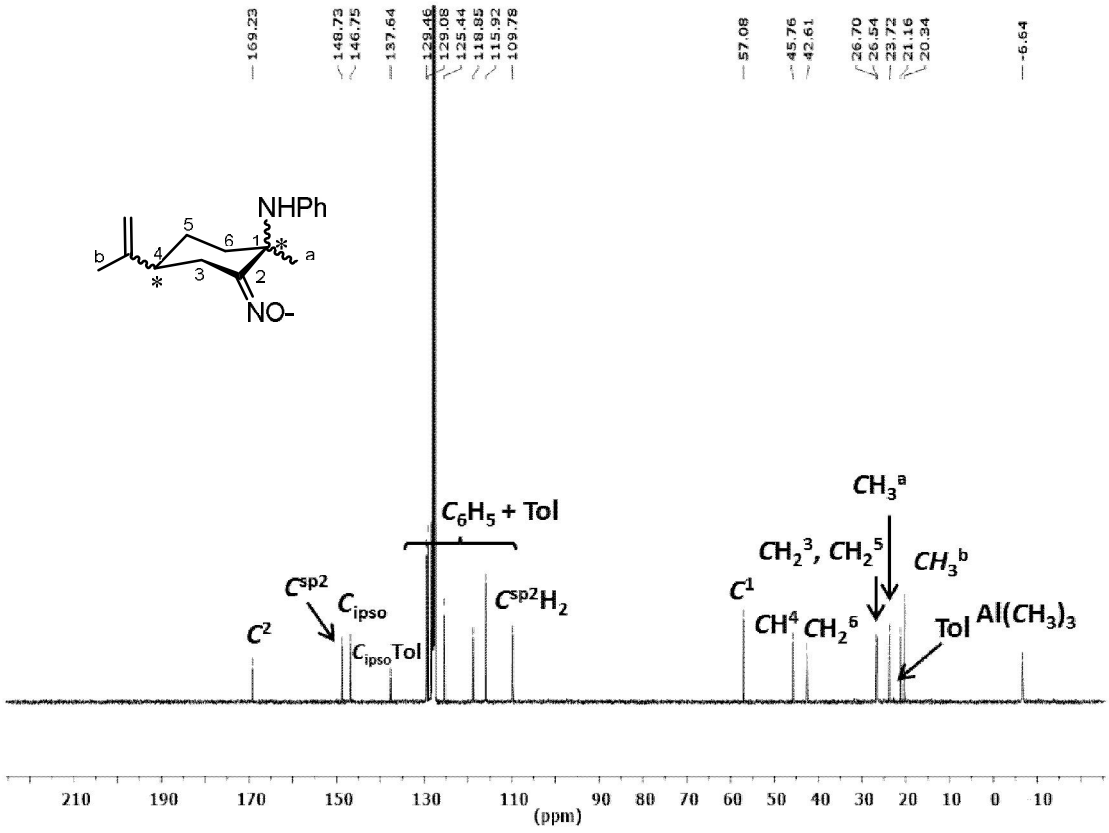


Figure S8. ^{13}C NMR (298K, C_6D_6, 100.62 MHz) spectrum for crystals of **(1*S*,4*R*)-1a** and **(1*R*,4*S*)-1a.**

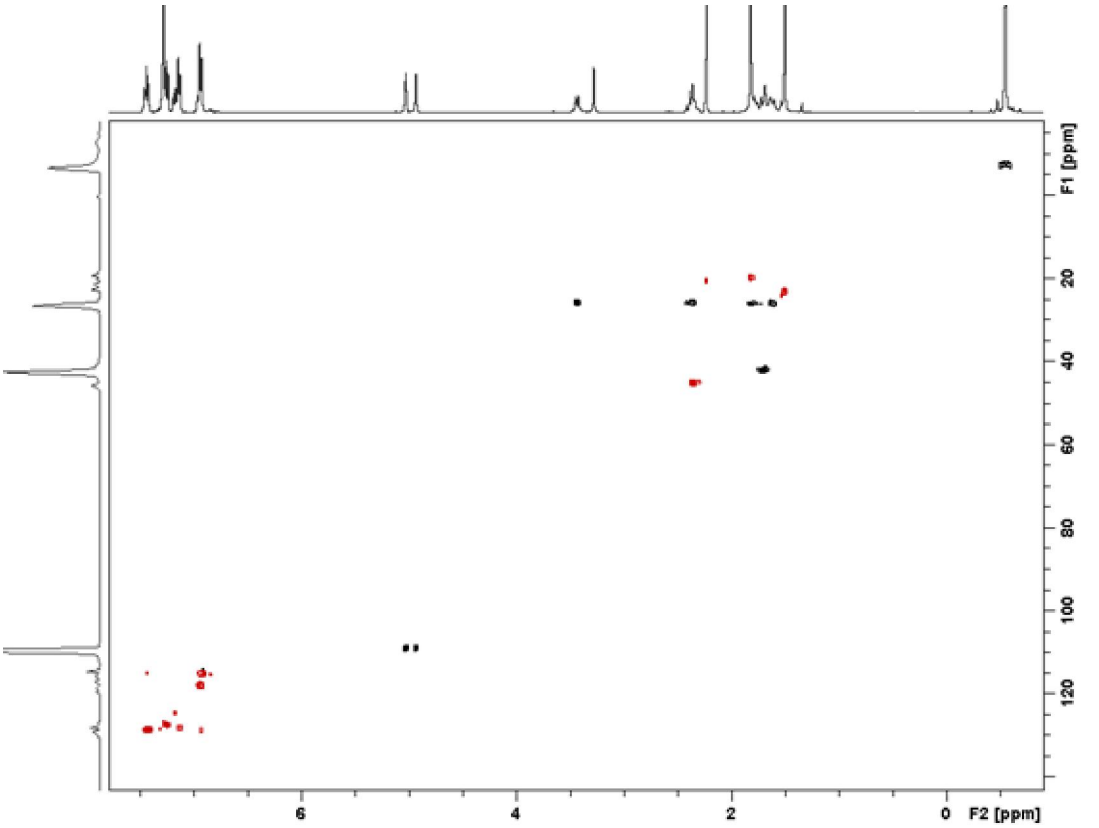


Figure S9. ^{1}H-^{13}C HSQC-*ed* NMR (298K, C_6D_6) spectrum for crystals of **(1*S,4R*)-1a** and **(1*R,4S*)-1a. Note:** Red signals correspond to CH and CH_3 groups. Black signals correspond to CH_2 groups.

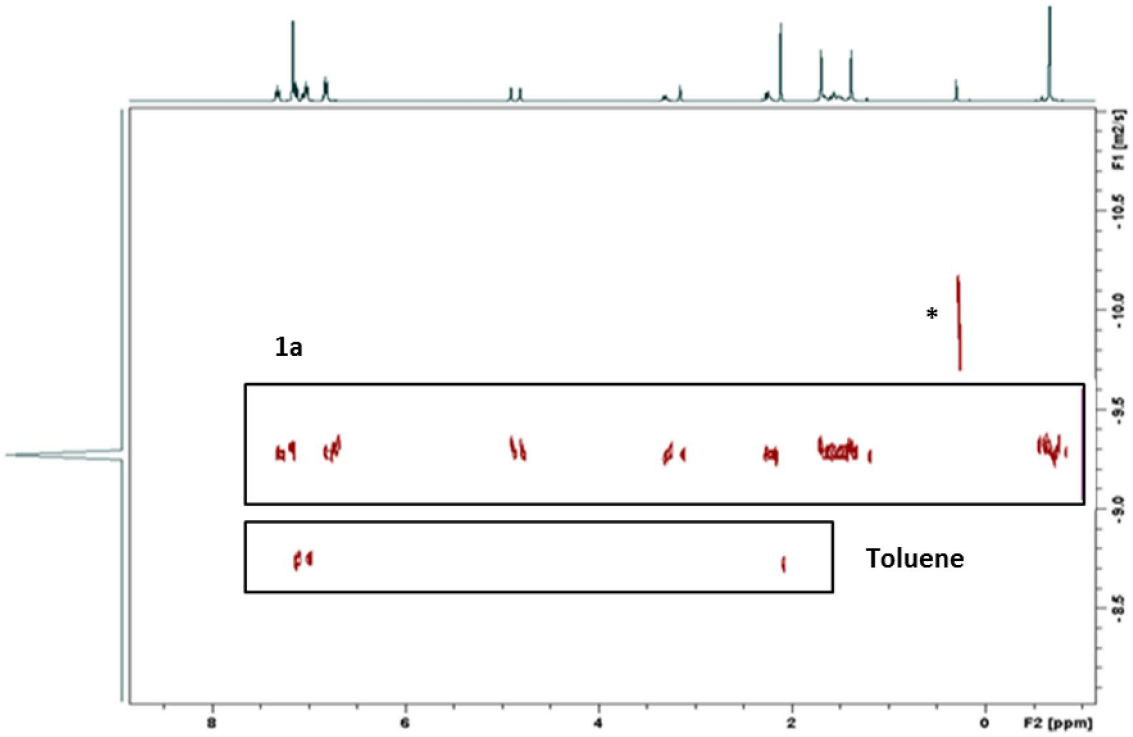


Figure S10.2D ^{1}H-DOSY NMR (298K, C_6D_6, 400.13 MHz) spectrum for crystals of **(1*S,4R*)-1a** and **(1*R,4S*)-1a.*** Represents grease

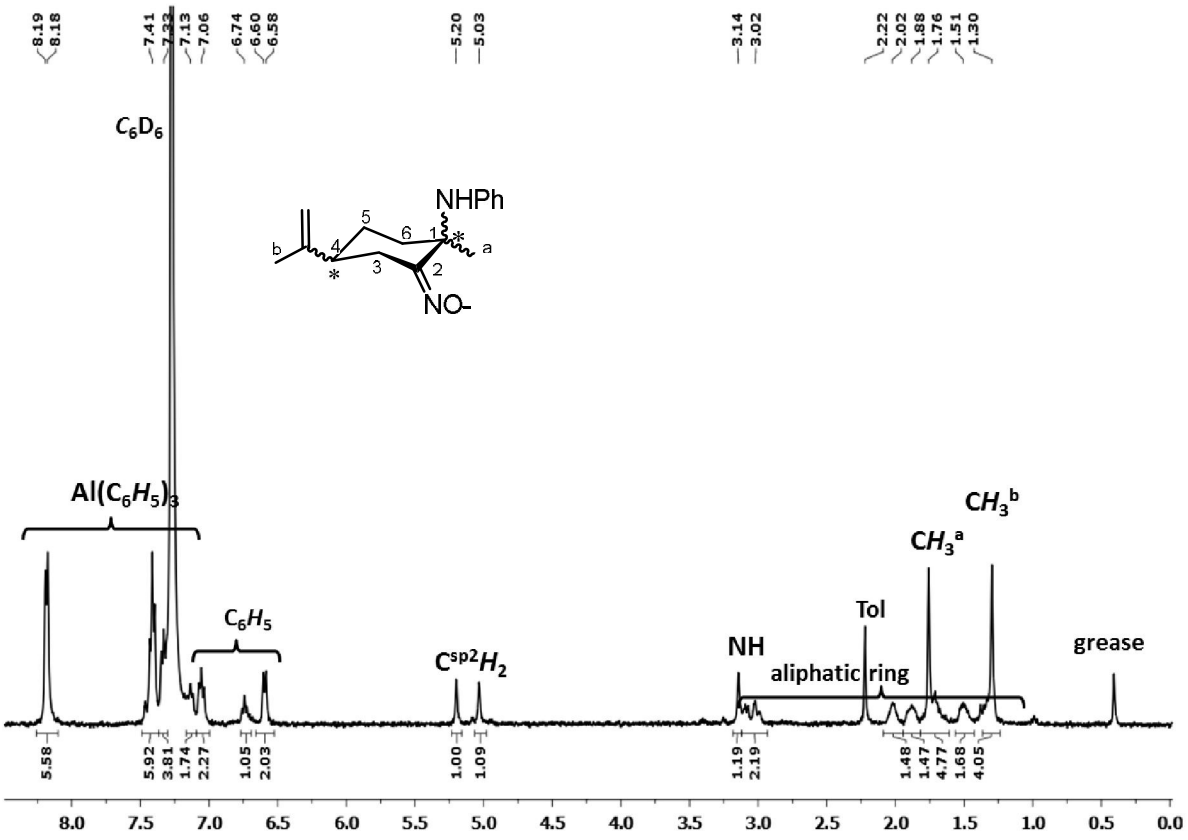


Figure S11. ^{1}H NMR (298K, C_6D_6, 400.13 MHz) spectrum for crystals of **(1*S*,4*R*)-1b.**

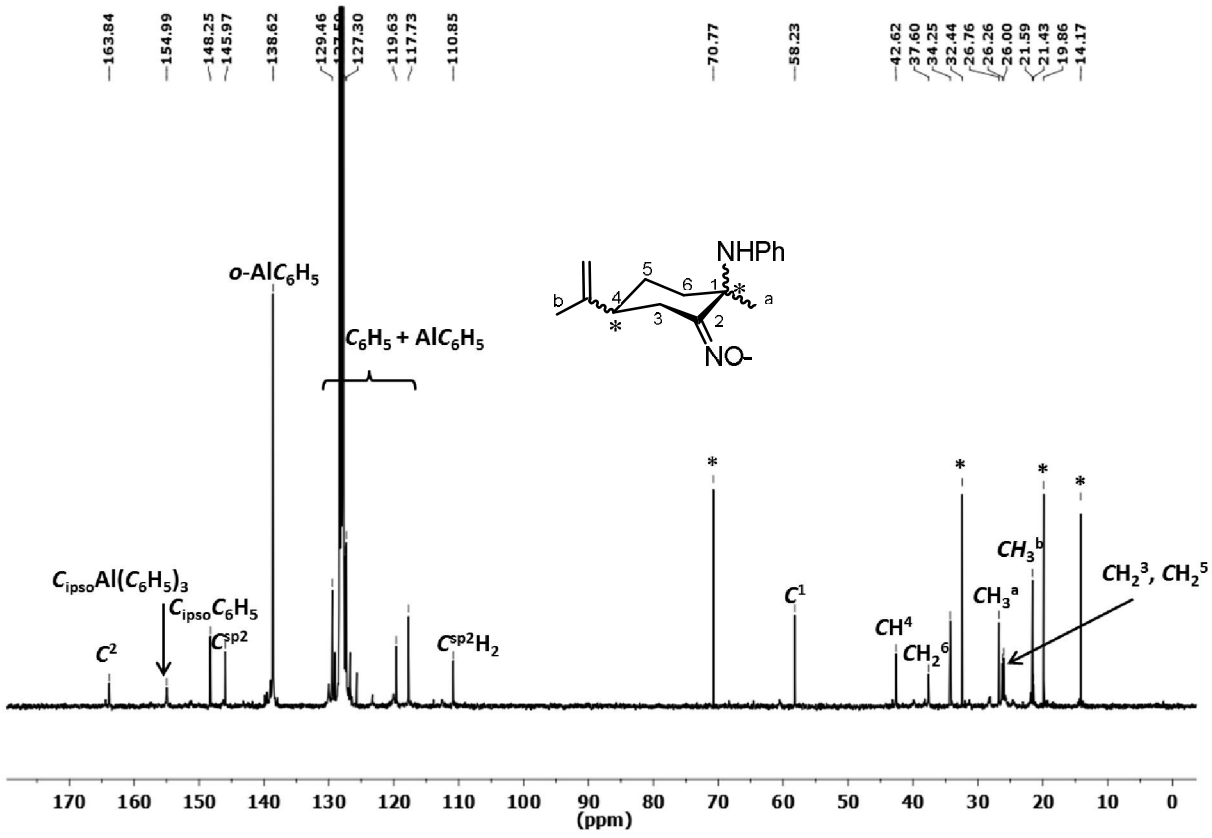


Figure S12. ^{13}C NMR (298K, C_6D_6, 100.62 MHz) spectrum for the reaction mixture of **(1*S*,4*R*)-1b.*** Represents Bu_2O as solvent of $AlPh_3$.

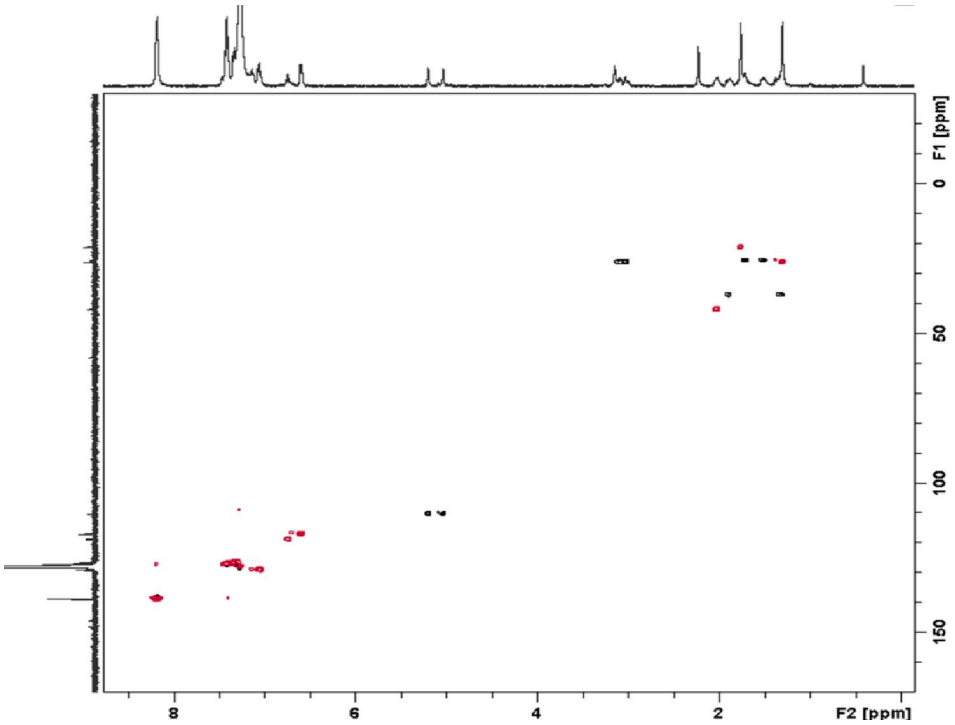


Figure S13. ^{1}H-^{13}C HSQC-*ed* NMR (298K, C_6D_6) spectrum for crystals of **(1*S*,4*R*)-1b**. **Note:** Red signals correspond to CH and CH_3 groups. Black signals correspond to CH_2 groups.

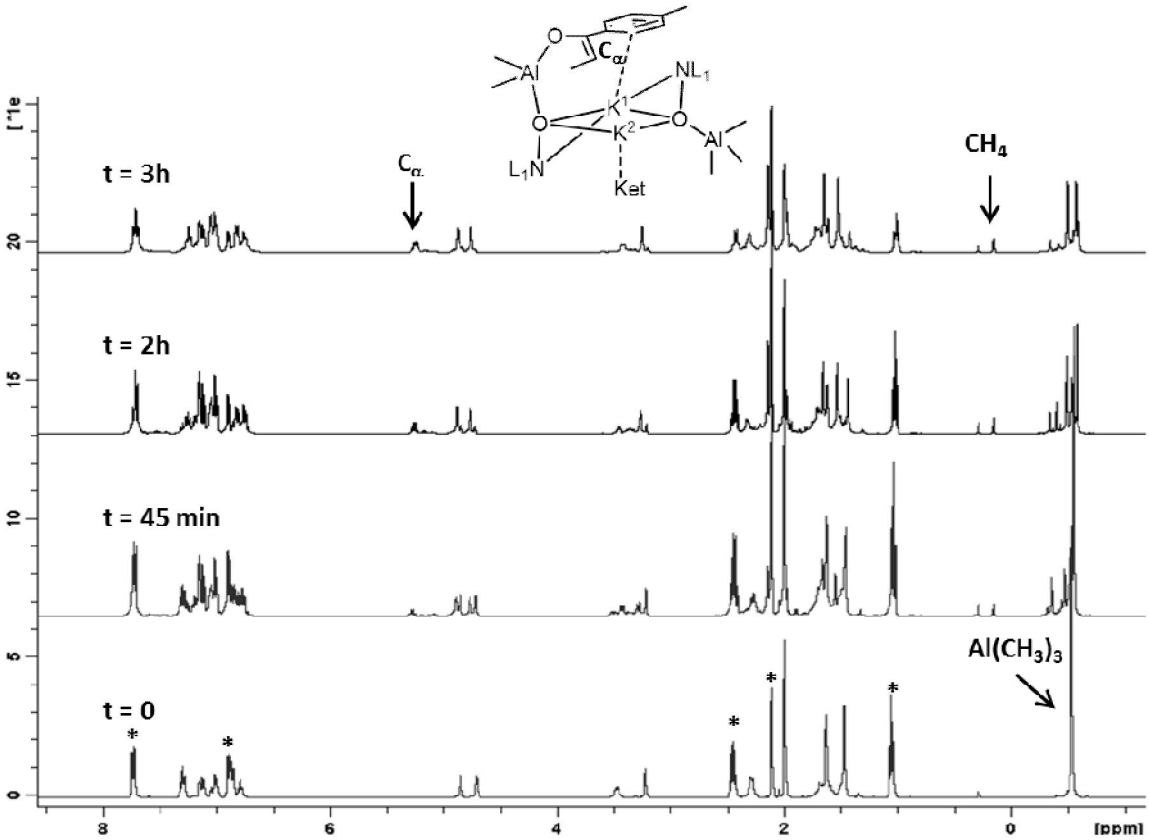


Figure S14. ^{1}H NMR (298K, C_6D_6, 400.13 MHz) monitoring of **(1*S*,4*R*)-1a** and *p*-methylpropiophenone reaction. * Represents *p*-methylpropiophenone. The formation of **2** and CH_4 is observed from t = 30 min.

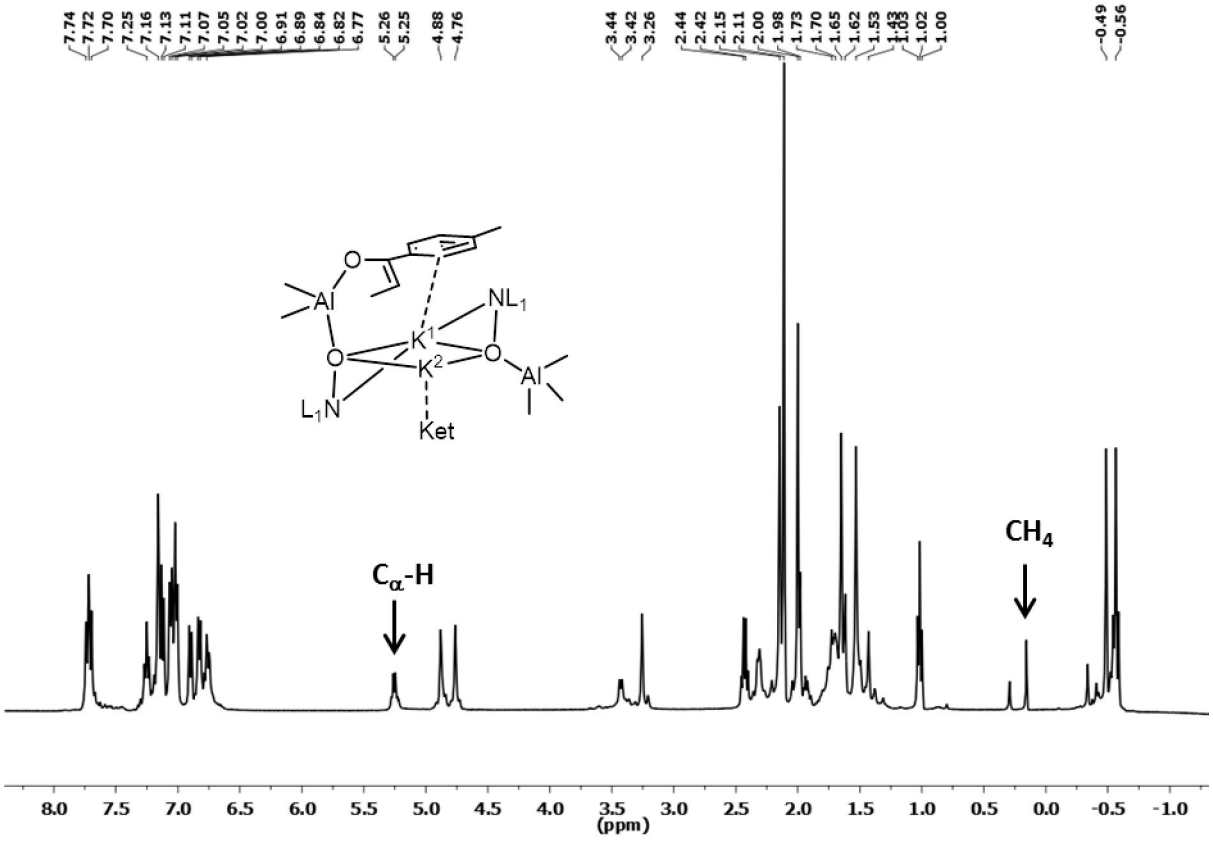


Figure S15. ^{1}H NMR (298K, C_6D_6, 400.13 MHz) spectrum for the *in situ* reaction of **1a** with 2 equivalents of 4-methylpropiophenone in C_6D_6.

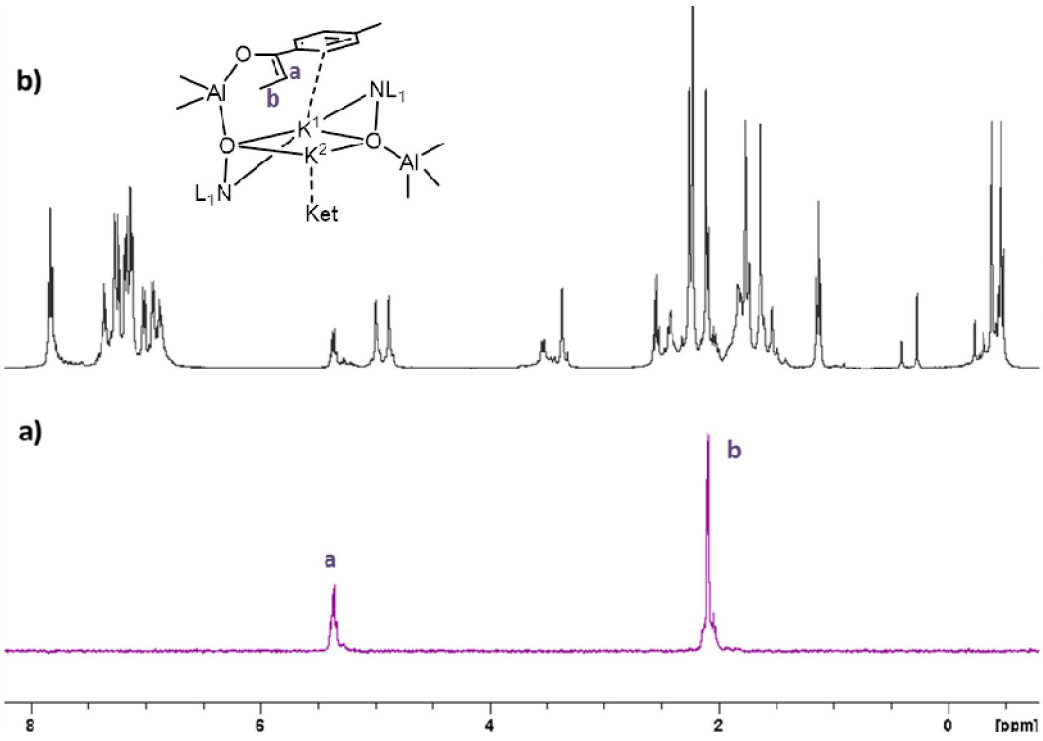


Figure S16.a) ^{1}H TOCSY NMR , b) ^{1}H NMR (298K, C_6D_6, 400.13 MHz) spectra of **2**. The TOCSY experiment allows to identify the resonance for C^{b}.

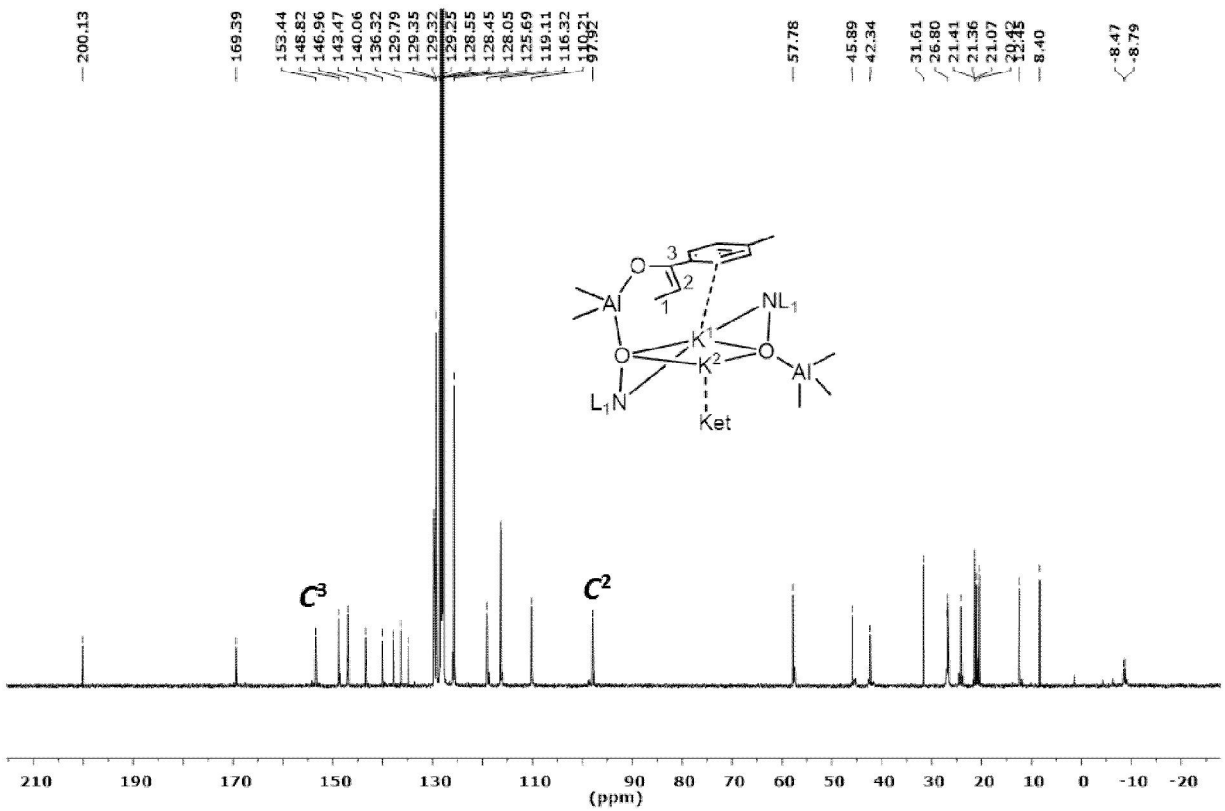


Figure S17. ^{13}C NMR (298K, C_6D_6, 100.62 MHz) spectra of **2** in C_6D_6.

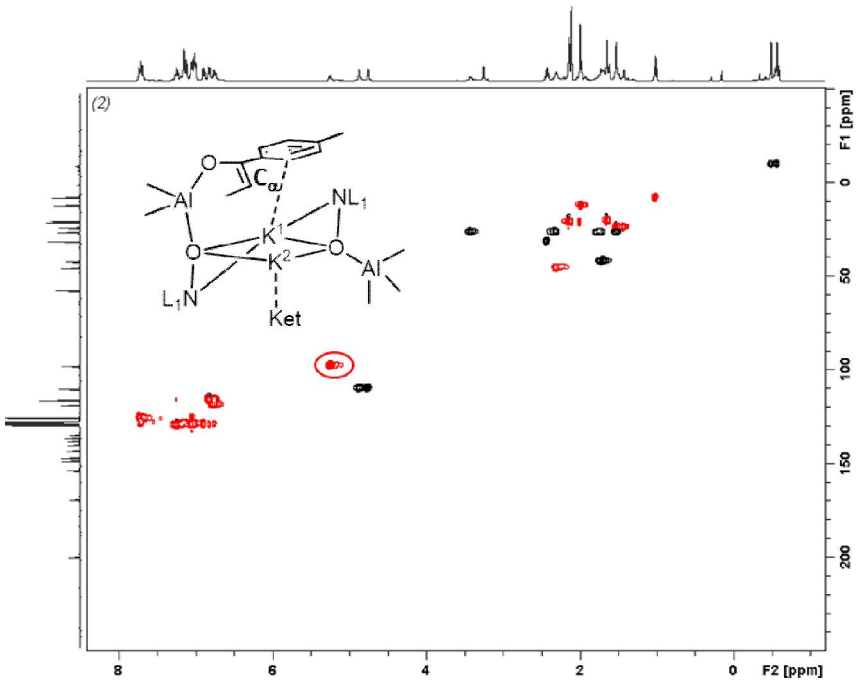


Figure S18. ^{1}H-^{13}C HSQC-*ed* NMR (298K, C_6D_6) spectrum of **2** in C_6D_6. **Note:** Red signals correspond to CH and CH_3 groups. Black signals correspond to CH_2 groups. The C_α signal corresponds to CH signal (red).

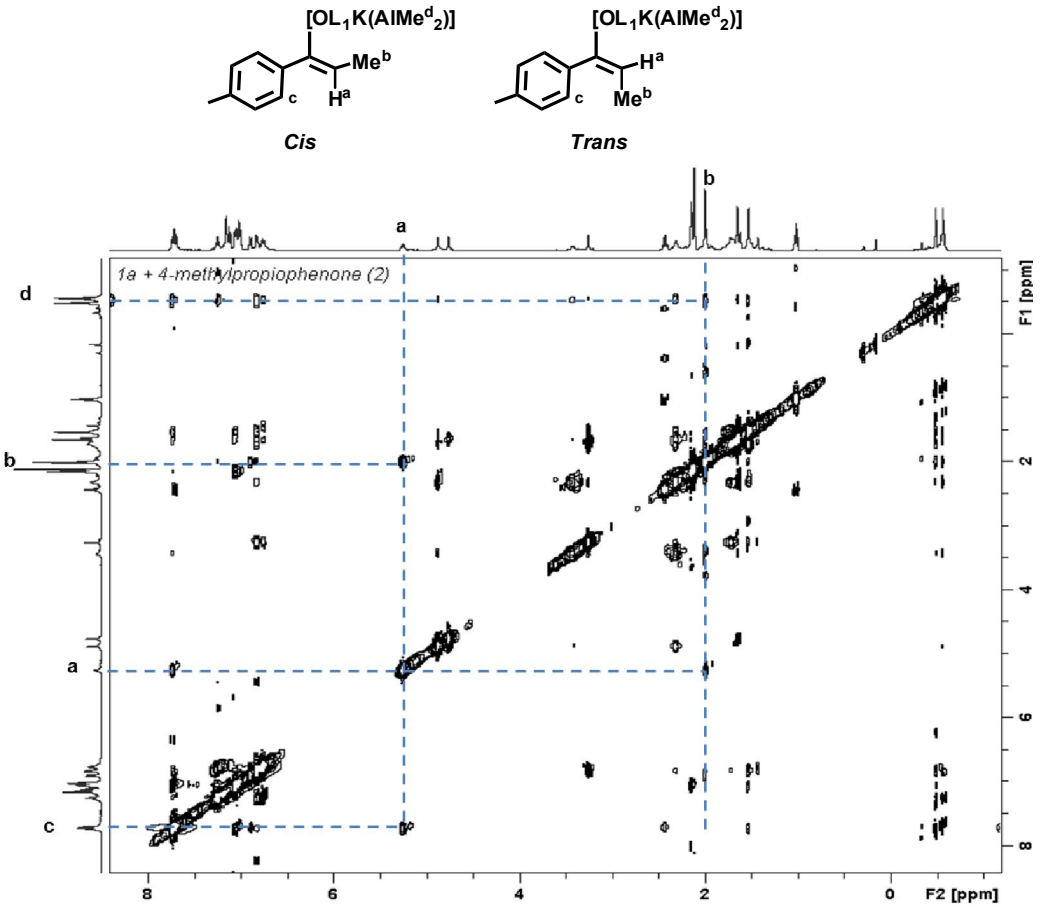


Figure S19. ^{1}H-^{1}H NOESY NMR (298K, C_6D_6, 400.13 MHz) spectrum of **2**. The *cis* isomer is the one observed.

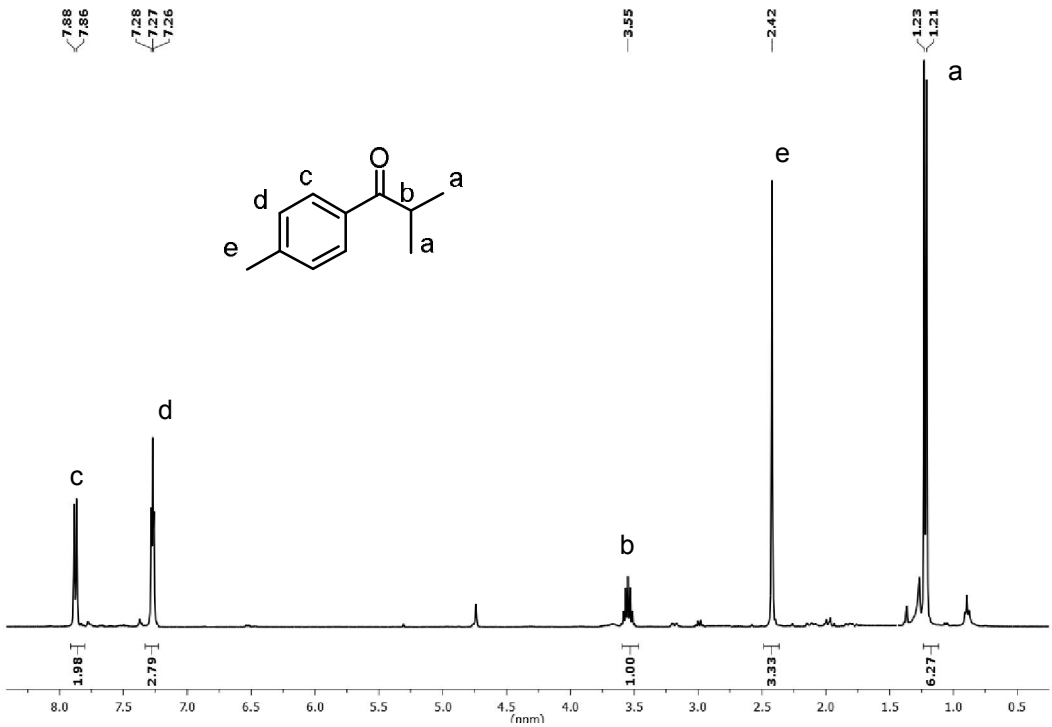


Figure S20. ^{1}H NMR (298K, $CDCl_3$, 400.13 MHz) spectrum of **4**.

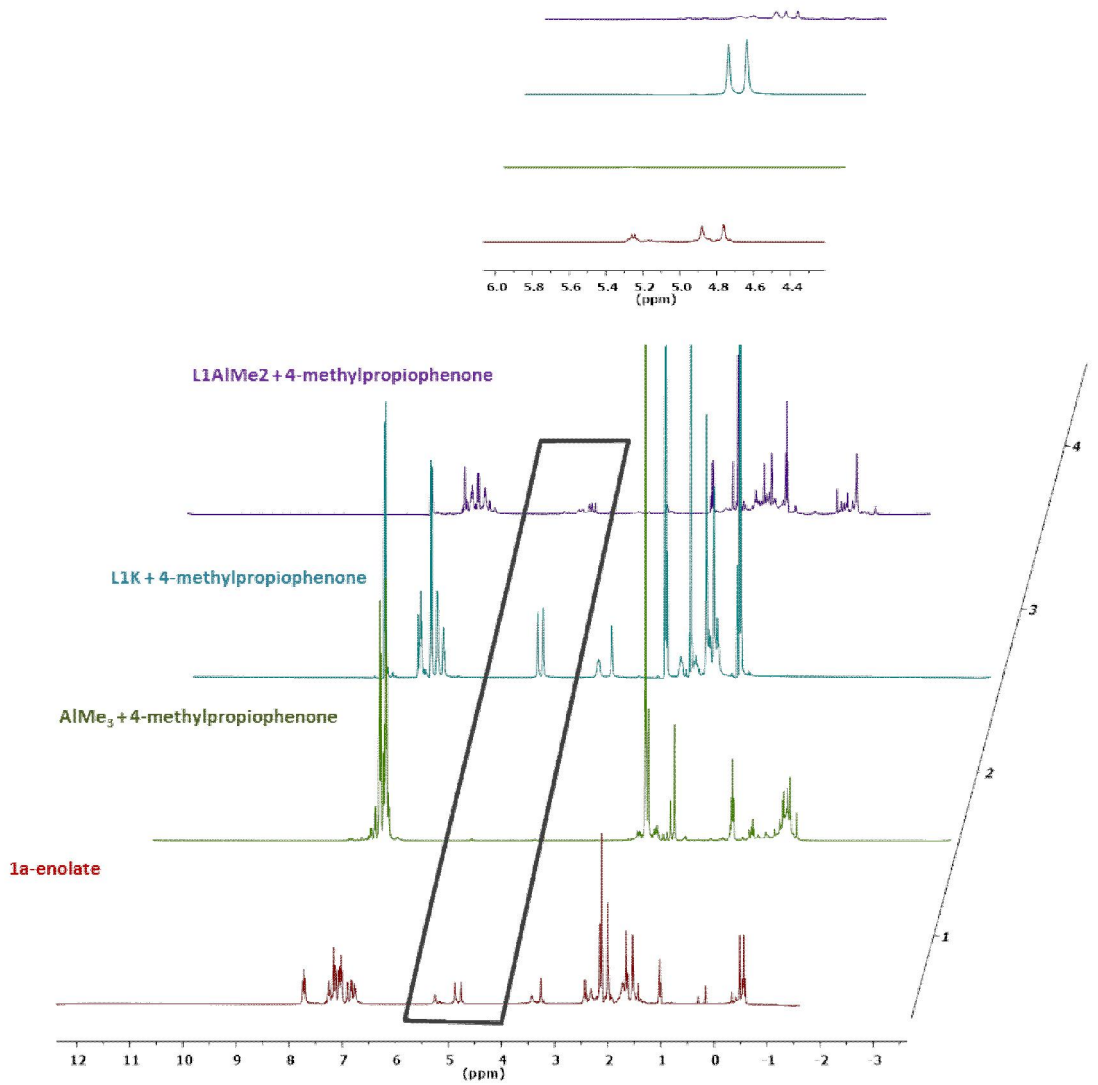


Figure S21. ^{1}H NMR (298K, C_6D_6, 400.13 MHz) spectrum of (from bottom to top): 1a-enolate, reactions of 4-methylpropiophenone vs $AlMe_3$, potassium oximate and aluminum oximate derivatives. As shown, the enolate is not formed when the homometallic species are used.

III. Diffusion-Ordered NMR Spectroscopy (DOSY) experiments

In Diffusion-Ordered NMR Spectroscopy (DOSY) experiments, a series of pulsed field gradient (PFG) stimulated echo experiments is performed and the results allow to generate a two dimensional spectrum where signals are dispersed depending on their diffusion coefficients. Since the diffusion coefficients (D) are related to the molecular size and shape of the molecules, a number of empirical methods for relating D to the molecular weight have been proposed based mainly in the dependence with the hydrodynamic radius of the molecule given by the Stokes-Einstein equation $D = kT/(6\pi\eta r_H)$, where k is the Boltzman constant, T is the temperature, η is the viscosity, and r_H is the hydrodynamic radius.[2] For small organometallic molecules the Li and Williard described a methodology that have successfully used by several groups. [3] In this approach, from the experimental data a calibration curve with at least three internal references to one NMR sample is generated, and the MW of the problem molecule (analyte) is calculated by interpolation.[4] However, recently Prof. Dietmar Stalke has reported a new methodology that overcomes the need of internal references by using external references to estimate the MW of the new species.[5]

Following this method we have estimated the MW of compounds **(1*S*,4*R*)-1a, (1*S*,4*R*)-1b** and **2** in solution. In all our samples TPhN was used as reference molecule. All samples were prepared in C_6D_6 by adding of 1,2,3,4-tetraphenylnaphthlene-TPhN (432.19 g mol^{-1}) and the analyte (each 15mM,) in an equimolar ratio. NMR experiments were carried out on a Bruker AV400 spectrometer equipped with a probe PABBO BB-1H/D Z-GRD. The diffusion time was $\Delta = 0.1$ s. The duration of the magnetic eld pulse gradients $\delta/2$ was adjusted for each molecule in a range of 1000–1600 ms. The delay for gradient recovery was 0.2 ms and the eddy current delay 5 ms. For each DOSY-NMR experiment, a series of 16 spectra on 32 K data points were collected. The pulse gradients (g) were incremented from 2 to 98% of the maximum gradient strength in a linear ramp with a total experiment time of 45 min. After Fourier transformation and baseline correction, the diffusion dimension was processed with the Topspin 2.0 software. Diffusion coefficients were calculated by Gaussian fits with the T1/T2 software of Topspin.

The values obtained for the diffusion coefficients were normalized in relation to the external reference using the equation (1)

$$\text{lod}\, D_{\text{x,norm}} = \log D_{\text{ref,fix}} - \log D_{\text{ref}} + \log D_{\text{x}} \qquad \textbf{(1)}$$

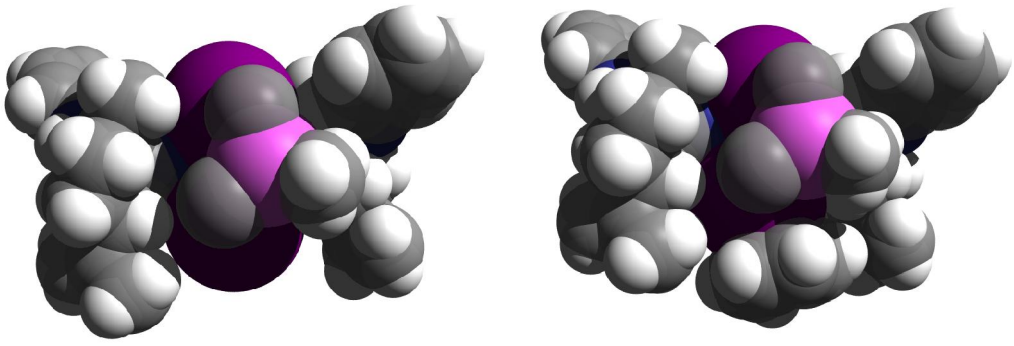
The MW values were calculated using equation (**2**), where *K* and α parameters depending on the compound geometry.

$$\text{MW}_{det} = 10^{\left(\frac{\log D_{x,norm} - \log K}{a}\right)} \qquad \textbf{(2)}$$

For **(1*S*,4*R*)-1a** and **(1*S*,4*R*)-1b**, the geometry considered was ECC_{DSE} based on its solid state structure (figure S-17). For compound **2** parameters corresponding to DSE and CS geometry were used respectively since a better agreement was achieved with the experimental data.

Table S1 [a] ECC_{DSE}^{TOL} was used to calculate the MW. [b]ECC_{CS}^{TOL} was used to calculate the MW.

Analyte	MW [g mol^{-1}]	MW_{det} [g mol^{-1}]	ΔMW [%]
(1*S*,4*R*)-1a [a]	737.078	680.64	7
(1*S*,4*R*)-1b [a]	1108.46	1075.58	-9
2[b]	1000.48	1076.23	-8



a) **b)**

Figure S22. a) Spacefill representation for **(1*S*,4*R*)-1a** molecular structure without the toluene molecules coordinated. b) Spacefill representation for **(1*S*,4*R*)-1a** molecular structure with on toluene molecule coordinated to the potassium atom.

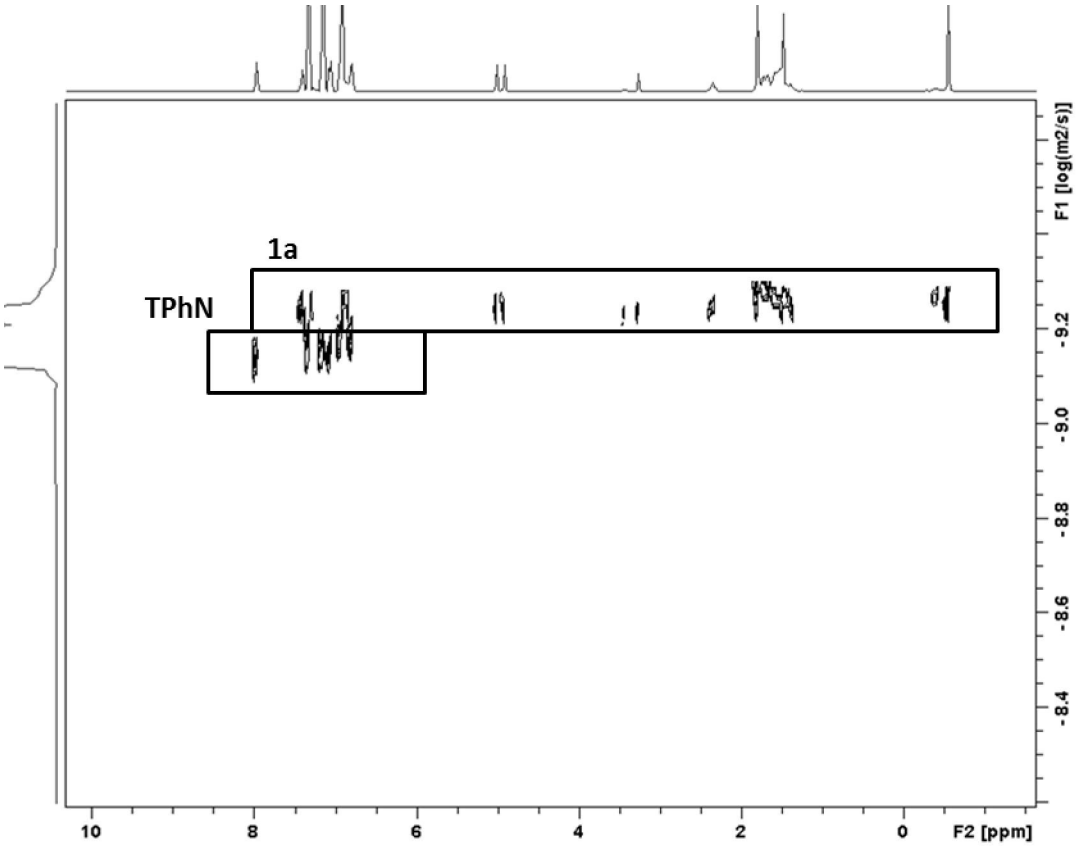


Figure S23. 2D ^{1}H DOSY NMR experiment of the mixture of TPhN and **1a** in C_6D_6.

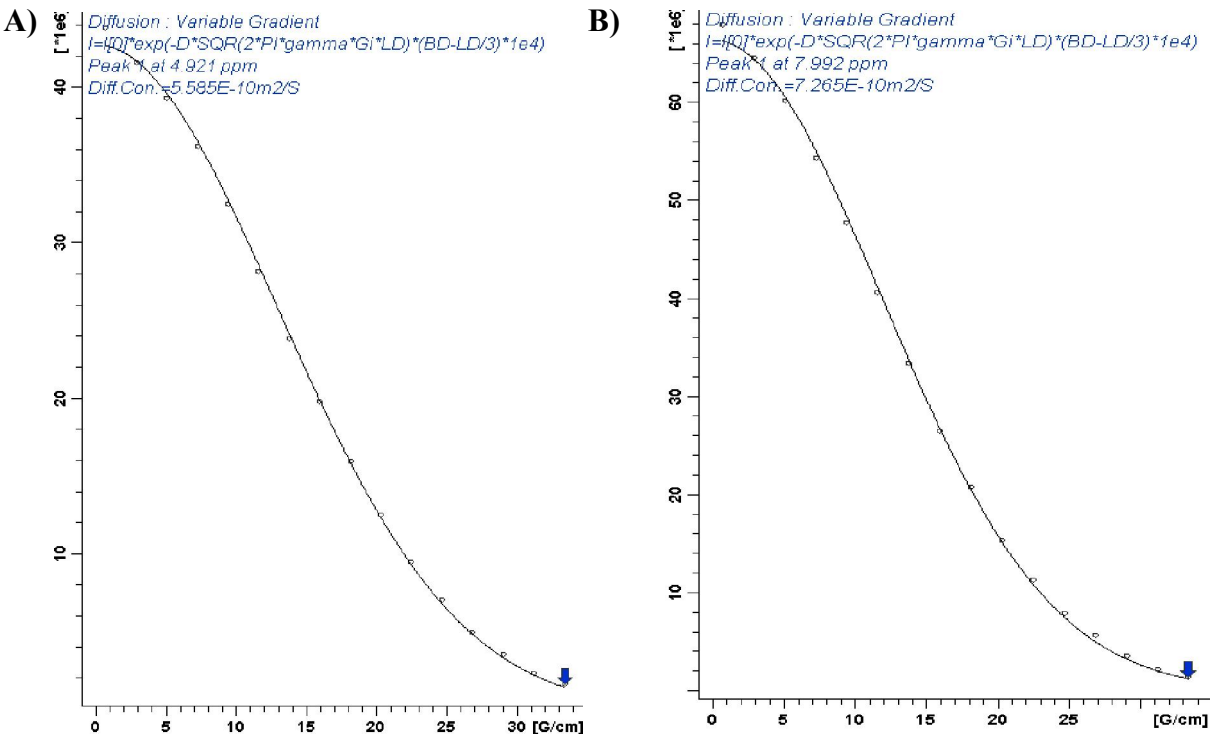


Figure S24. A) Gaussian fits of **1a** in C_6D_6. **B)** Gaussian fits of **TPhN** in C_6D_6.

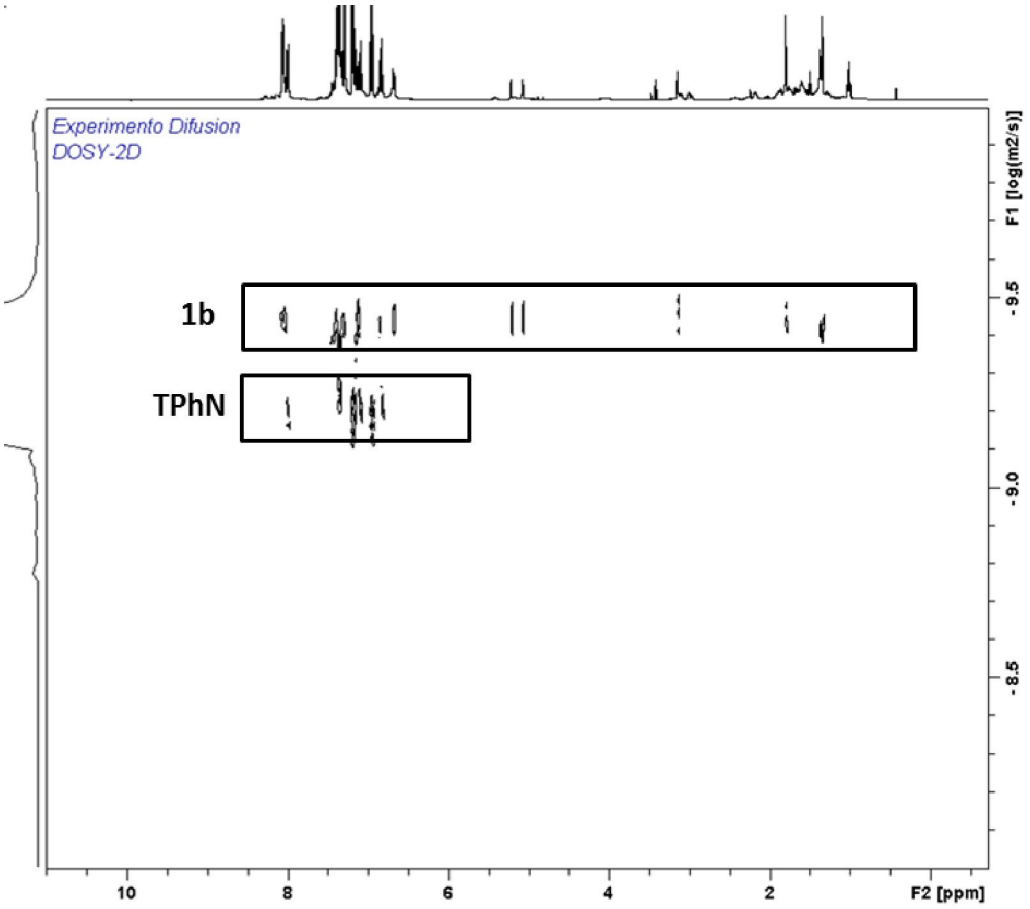


Figure S25. 2D ^{1}H-DOSY NMR experiment of the mixture of TPhN and **1b** in C_6D_6.

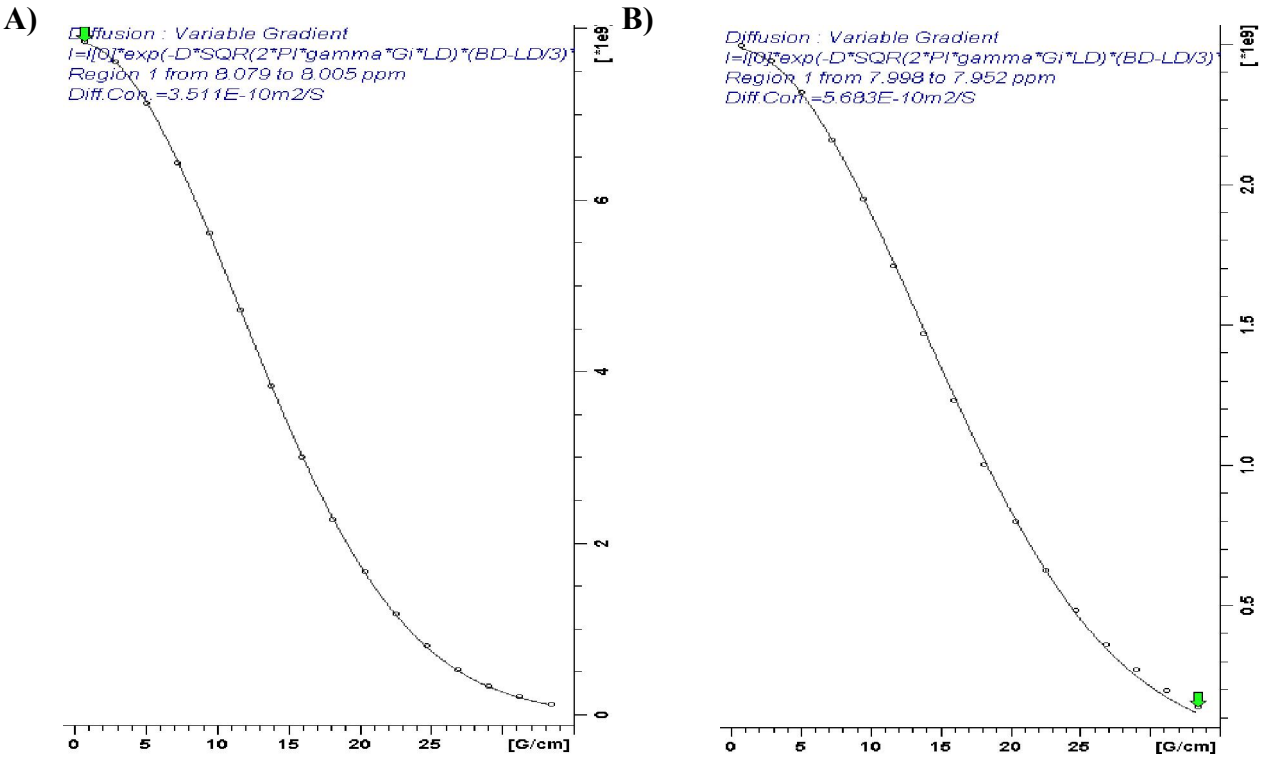


Figure S26. A) Gaussian fits of **1b** in C_6D_6. **B)** Gaussian fits of **TPhN** in C_6D_6.

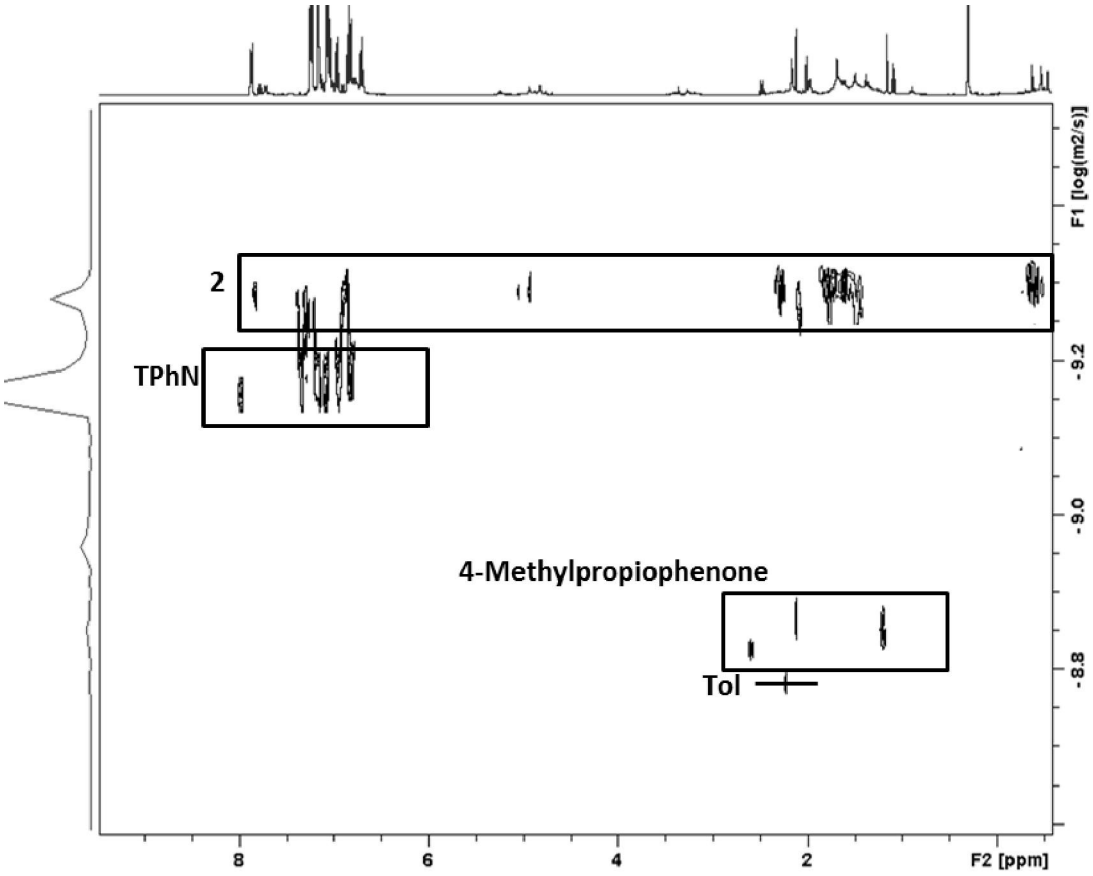


Figure S27. 2D ^{1}H-DOSY NMR experiment of the mixture of TPhN and **2** in C_6D_6.

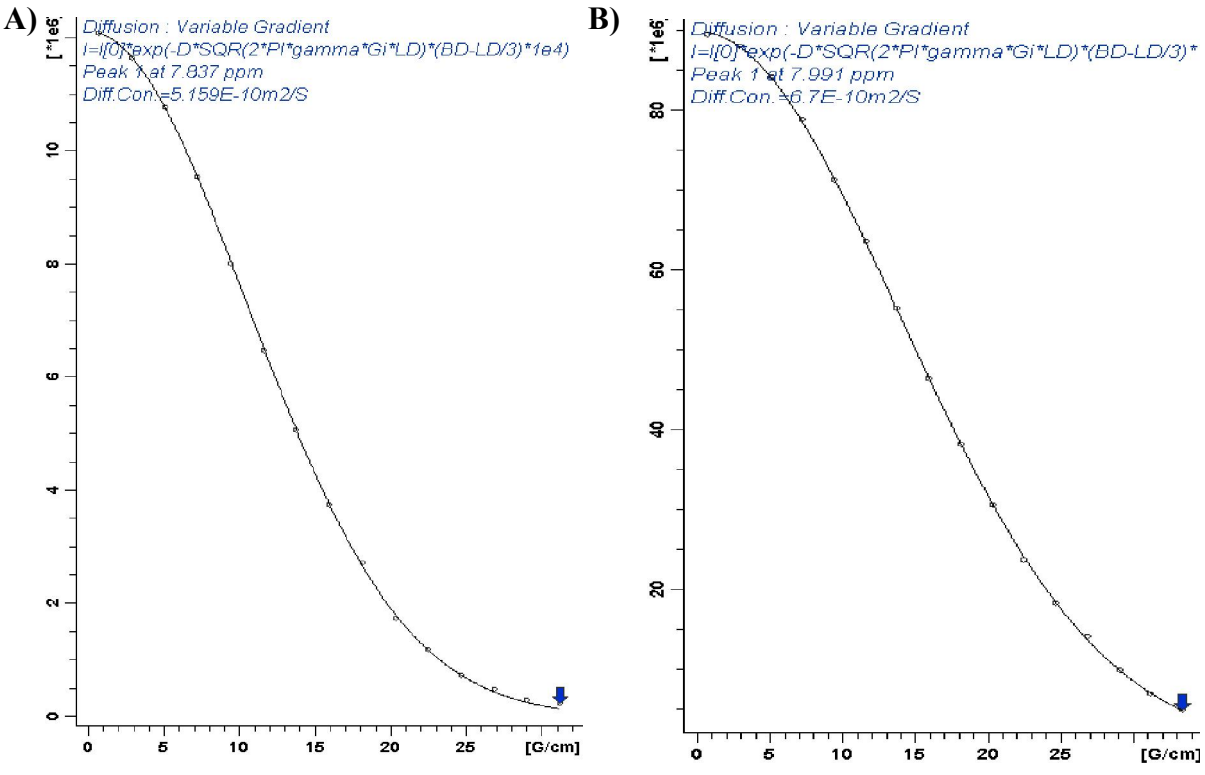


Figure S28. A) Gaussian fits of **2** in C_6D_6. **B)** Gaussian fits of **TPhN** in C_6D_6.

IV. Single-Crystal X-ray Structure Determination of Compounds (1*S*,4*R*)-1a·C_6D_6, (1*R*,4*S*)-1a·C_6D_6, (1*S*,4*R*)-1c·0.5(C_7H_8·C_6D_6) and 3 C_6D_6.

Details of the X-ray experiment, data reduction, and final structure refinement calculations are summarized in Table S-2. Suitable single crystals of **(1*S*,4*R*)-1a·C_6D_6**, **(1*R*,4*S*)-1a·C_6D_6**, **(1*S*,4*R*)-1c·0.5(C_7H_8·C_6D_6)** and **3 C_6D_6** for the X-ray diffraction study were selected. Data collection was performed at 200(2) K, with the crystals covered with perfluorinatedether oil. The crystals were mounted on a Bruker-Nonius Kappa CCD single crystal diffractometer equipped with a graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å). Multiscan[6] absorption correction procedures were applied to the data. The structures were solved, using the WINGX package,[7] by direct methods (SHELXS-97) and refined using full-matrix least-squares against F^2 (SHELXL-14).[8] Full-matrix least-squares refinements were carried out by minimizing $\Sigma w(F_o^2-F_c^2)^2$ with the SHELXL-14 weighting scheme and stopped at shift/err < 0.001. All non-hydrogen atoms were anisotropically refined and hydrogen atoms were geometrically placed and left riding on their parent atoms except for:.

For **(1*S*,4*R*)-1a·C_6D_6** the hydrogen atoms bonded to N11 and N21 were found in the Fourier map and freely refined. Hydrogen atoms on C1, C2, C5 and C6 (that corresponds to the methyl groups that show an interaction with the potassium atoms), were not possible to be geometrically placed or to be modeled from the Fourier map. One carbon atom (C75) from the toluene coordinated to K1 was disorder but the disorder was not treated. One molecule of deuterated benzene per molecule of compound was found in the difference Fourier map but was very disordered and it was not possible to get a chemically sensible model for it, so the Squeeze procedure[9] was used to remove its contribution to the structure factors.

For **(1*R*,4*S*)-1a·C_6D_6** data quality was very poor, so C12 and C44 were left isotropic. Hydrogen atoms on C1, C2, C5 and C6 (that corresponds to the methyl groups that show an interaction with the potassium atoms), were not possible to be geometrically placed or to be modeled from the Fourier map. Three carbon atoms from the toluene molecules coordinated were disordered (C63, C72, C73) but the disorder was not treated. Some restrains (FLAT) were applied to the phenyl group (C41>C46) bonded to N21. As well one molecule of deuterated benzene per molecule of compound was found in the difference Fourier map but was very disordered and it was not possible to get a

chemically sensible model for it, so the Squeeze procedure[9] was used to remove its contribution to the structure factors

For the **(1*S*,4*R*)-1c·0.5(C_7H_8·C_6D_6)**, there is one C_6D_6 and one toluene molecule per two molecules of the compound. The molecule of C_6D_6 shows an interaction with the compound **(1*S*,4*R*)-1c·0.5(C_7H_8·C_6D_6)** and it was possible to be modeled, however the toluene molecule was not possible to make chemical sense of it so Squeeze procedure was applied.[9] C60, C65 and C75 from the coordinated benzene rings were disorder but the disordered was not treated. The hydrogen atoms for C1, C2, C5 and C6, that correspond to the methyl groups that show an interaction with the potassium atoms, and the hydrogen bonded to N11 and N21 were found in the Fourier map and freely refined. The enantiomer **(1*R*,4*S*)-1b·0.5(C_7H_8·C_6D_6)**, was identified by the coincidence with the unit cell with **(1*S*,4*R*)-1b·0.5(C_7H_8·C_6D_6)**but no data were taken.

Table S2. Crystallographic Data for **(1*S*,4*R*)-1a·C_6D_6**, **(1*R*,4*S*)-1a·C_6D_6**, **(1*S*,4*R*)-1c·0.5(C_7H_8·C_6D_6)** and **3 C_6D_6**.

	(1*S*,4*R*)-1a·C_6D_6	**(1*R*,4*S*)-1a·C_6D_6**	**(1*S*,4*R*)-1c·0.5 (C_7H_8·C_6D_6)**	**3·C_6D_6**
Empirical formula	$C_{52}H_{77}Al_2K_2N_4O_2 \cdot C_6D_6$	$C_{52}H_{77}Al_2K_2N_4O_2 \cdot C_6D_6$	$C_{50}H_{60}Al_2D_{12}K_2N_4O_2 \cdot 0.5\ C_7H_8\ C_6D_6$	$C_{28}H_{26}AlKO \cdot C_6D_6$
Formula weight	1006.48	1006.48	993.48	528.71
Color, shape	colorless/block	colorless/block	colorless/block	colorless/block
Crystal size (mm)	0.46x0.41x0.32	0.38x0.27x0.15	0.48x0.45x0.42	0.32x0.23x0.11
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Monoclinic
Space group	$P2_12_12$	$P2_12_12$	$P2_12_12$	$P2_1/n$
a (Å)	11.9997(17)	32.214(11)	31.579(5)	9.3304(19)
b (Å)	32.297(9)	11.964(8)	11.8642(11)	22.004(7)
c (Å)	15.606(7)	15.575(14)	15.4746(14)	14.487(4)
β (deg.)	90	90	90	92.699(19)
V (Å^3)	6048(3)	6003(7)	5797.8(12)	2971.0(14)
Z	4	4	4	4
T(K)	200	200	200	200
$\rho_{calcd.}$ (mg m^{-3})	1.105	1.114	1.138	1.182
F_{000}	2156	2156	2104	1104
λ (Å)	0.71073	0.71073	0.71073	0.71073
μ (mm^{-1})	0.226	0.228	0.235	0.232
θ Range (°)	3.114 to 23.520	3.049 to 19.997	3.099 to 26.899	3.114 to 24.998
Data collected (h,k,l)	±13, ±36, ±17	±30, ±11, ±14	±40, ±15, ±19	±11, ±26, ±17
Reflns. collected	55741	92427	66701	19633
Indep. Reflns./Rint	8910 / 0.1287	5580 / 0.1692	12414 / 0.0669	5217 / 0.1341
Data/restraints/param	8910 / 0 / 567	5580 / 3 / 549	12414 / 0 / 624	5217 / 0 / 350
R_1/wR_2 (I > 2σ(I))[a]	0.0790 / 0.2060	0.0998 / 0.2245	0.0584/ 0.1398	0.0720 / 0.1425
R_1/wR_2 (all data)[a]	0.1028 / 0.2251	0.1572 / 0.2563	0.0820 / 0.1540	0.1551 / 0.1648
Flack parameter	-0.03(4)	-0.02(5)	0.00(2)	
GOF	1.011	1.014	1.045	1.026
Max/min Δρ (e.Å^{-3})	0.318 / -0.289	0.323 / -0.281	0.298 / -0.249	0.247 / -0.170

[a] $R_1 = \Sigma(||F_o| - |F_c||)/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; GOF = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)\}^{1/2}$.

Table S3. Selected bond lengths [Å] and angles [deg] for **(1*S*,4*R*)-1a·C_6D_6**, **(1*R*,4*S*)-1a·C_6D_6** and **(1*S*,4R)-1c·0.5(C_7H_8·C_6D_6)**

(1*S*,4*R*)-1a·C_6D_6		**(1*R*,4*S*)-1a·C_6D_6**		**(1*S*,4*R*)-1c·0.5(C_7H_8·C_6D_6)**	
BONDS (Å)					
Al(1)-O(2)	1.828(6)	Al(1)-O(2)	1.804(13)	Al(1)-O(2)	1.833(3)
Al(1)-C(1)	2.007(9)	Al(1)-C(1)	2.01(2)	Al(1)-C(1)	1.981(6)
Al(1)-C(2)	2.003(9)	Al(1)-C(2)	1.99(2)	Al(1)-C(2)	1.969(6)
Al(1)-C(3)	1.990(9)	Al(1)-C(3)	2.03(2)	Al(1)-C(3)	1.965(5)
Al(2)-O(1)	1.835(6)	Al(2)-O(1)	1.824(12)	Al(2)-O(1)	1.829(3)
Al(2)-C(4)	1.983(10)	Al(2)-C(4)	1.99(2)	Al(2)-C(4)	1.970(6)
Al(2)-C(5)	1.999(11)	Al(2)-C(5)	2.002(19)	Al(2)-C(5)	1.983(7)
Al(2)-C(6)	2.005(11)	Al(2)-C(6)	2.01(2)	Al(2)-C(6)	1.983(7)
K(1)-N(1)	2.738(6)	K(1)-N(1)	2.724(14)	K(1)-N(1)	2.719(3)
K(1)-N(2)	2.734(6)	K(1)-N(2)	2.739(17)	K(1)-N(2)	2.733(3)
K(1)-O(1)	2.879(5)	K(1)-O(1)	2.994(12)	K(1)-O(1)	2.822(3)
K(1)-O(2)	3.009(5)	K(1)-O(2)	2.884(13)	K(1)-O(2)	3.039(3)
K(1)-C(2)	3.132(9)	K(1)-C(2)	3.13(2)	K(1)-C(2)	3.118(6)
K(1)-C(6)	3.117(10)	K(1)-C(6)	3.118(19)	K(1)-C(6)	3.178(7)
K(1)-C(70)	3.496(9)	K(1)···C(72)	3.56(2)	K(1)-C(70)	3.337(6)
K(1)-C(71)	3.470(9)	K(1)-C(72)	3.50(2)	K(1)-C(71)	3.380(5)
K(1)-C(72)	3.408(10)	K(1)-C(73)	3.46(2)	K(1)-C(72)	3.424(6)
K(1)-C(73)	3.418(11)	K(1)-C(74)	3.38(3)	K(1)-C(73)	3.433(6)
K(1)-C(74)	3.435(12)	K(1)-C(75)	3.35(2)	K(1)-C(74)	3.390(6)
K(1)-C(75)	3.455(10)	K(1)-C(76)	3.41(2)	K(1)-C(75)	3.341(6)
K(2)-O(1)	2.583(5)	K(2)-O(1)	2.546(12)	K(2)-O(1)	2.567(3)
K(2)-O(2)	2.574(5)	K(2)-O(2)	2.584(13)	K(2)-O(2)	2.565(3)
K(2)-C(1)	3.150(9)	K(2)-C(1)	3.13(2)	K(2)-C(1)	3.251(9)
K(2)-C(5)	3.135(12)	K(2)-C(5)	3.16(2)	K(2)-C(5)	3.171(8)
K(2)-C(60)	3.229(10)	K(2)-C(61)	3.26(2)	K(2)-C(60)	3.270(7)
K(2)-C(61)	3.138(9)	K(2)-C(62)	3.36(3)	K(2)-C(61)	3.165(6)
K(2)-C(62)	3.200(10)	K(2)-C(63)	3.41(3)	K(2)-C(62)	3.118(6)
K(2)-C(63)	3.326(11)	K(2)-C(64)	3.30(3)	K(2)-C(63)	3.186(6)
K(2)-C(64)	3.369(11)	K(2)-C(65)	3.15(2)	K(2)-C(64)	3.286(6)
K(2)-C(65)	3.336(11)	K(2)-C(66)	3.10(2)	K(2)-C(65)	3.330(7)
N(1)-O(1)	1.408(8)	N(1)-O(1)	1.406(16)	N(1)-O(1)	1.412(4)
N(1)-C(10)	1.277(9)	N(1)-C(10)	1.279(18)	N(1)-C(10)	1.283(5)
N(2)-O(2)	1.427(8)	N(2)-O(2)	1.451(17)	N(2)-O(2)	1.417(4)
N(2)-C(20)	1.279(9)	N(2)-C(39)	1.281(19)	N(2)-C(20)	1.266(5)
N(11)-C(11)	1.482(12)	N(11)-C(11)	1.431(19)	N(11)-C(11)	1.463(6)
N(11)-C(31)	1.422(15)	N(11)-C(26)	1.34(2)	N(11)-C(31)	1.395(7)
N(21)-C(21)	1.489(9)	N(21)-C(21)	1.47(2)	N(21)-C(21)	1.477(5)
N(21)-C(41)	1.396(9)	N(21)-C(46)	1.42(3)	N(21)-C(41)	1.387(6)
ANGLES (º)					
O(1)-K(1)-O(2)	74.03(14)	O(2)-K(1)-O(1)	73.5(3)	O(1)-K(1)-O(2)	74.11(8)
O(2)-K(2)-O(1)	86.87(17)	O(1)-K(2)-O(2)	86.6(4)	O(2)-K(2)-O(1)	87.10(9)
N(1)-O(1)-Al(2)	119.0(4)	N(1)-O(1)-Al(2)	117.4(9)	N(1)-O(1)-Al(2)	117.2(2)
N(1)-O(1)-K(2)	131.8(4)	N(1)-O(1)-K(2)	130.9(9)	N(1)-O(1)-K(2)	132.7(2)
Al(2)-O(1)-K(2)	109.0(2)	Al(2)-O(1)-K(2)	109.9(5)	Al(2)-O(1)-K(2)	110.06(13)
N(1)-O(1)-K(1)	70.0(3)	N(1)-O(1)-K(1)	65.3(7)	N(1)-O(1)-K(1)	71.20(18)
Al(2)-O(1)-K(1)	98.6(2)	Al(2)-O(1)-K(1)	95.4(5)	Al(2)-O(1)-K(1)	99.31(12)
K(2)-O(1)-K(1)	101.1(2)	K(2)-O(1)-K(1)	99.0(4)	K(2)-O(1)-K(1)	102.11(10)
N(2)-O(2)-Al(1)	118.3(4)	N(2)-O(2)-Al(1)	120.4(10)	N(2)-O(2)-Al(1)	117.7(2)
N(2)-O(2)-K(2)	129.5(4)	N(2)-O(2)-K(2)	130.0(9)	N(2)-O(2)-K(2)	127.2(2)

Al(1)-O(2)-K(2)	109.9(2)	Al(1)-O(2)-K(2)	109.5(6)	Al(1)-O(2)-K(2)	112.54(13)
N(2)-O(2)-K(1)	65.1(3)	N(2)-O(2)-K(1)	69.6(8)	N(2)-O(2)-K(1)	64.02(17)
Al(1)-O(2)-K(1)	94.8(2)	Al(1)-O(2)-K(1)	99.2(5)	Al(1)-O(2)-K(1)	95.51(12)
K(2)-O(2)-K(1)	97.97(16)	K(2)-O(2)-K(1)	100.9(4)	K(2)-O(2)-K(1)	96.56(9)

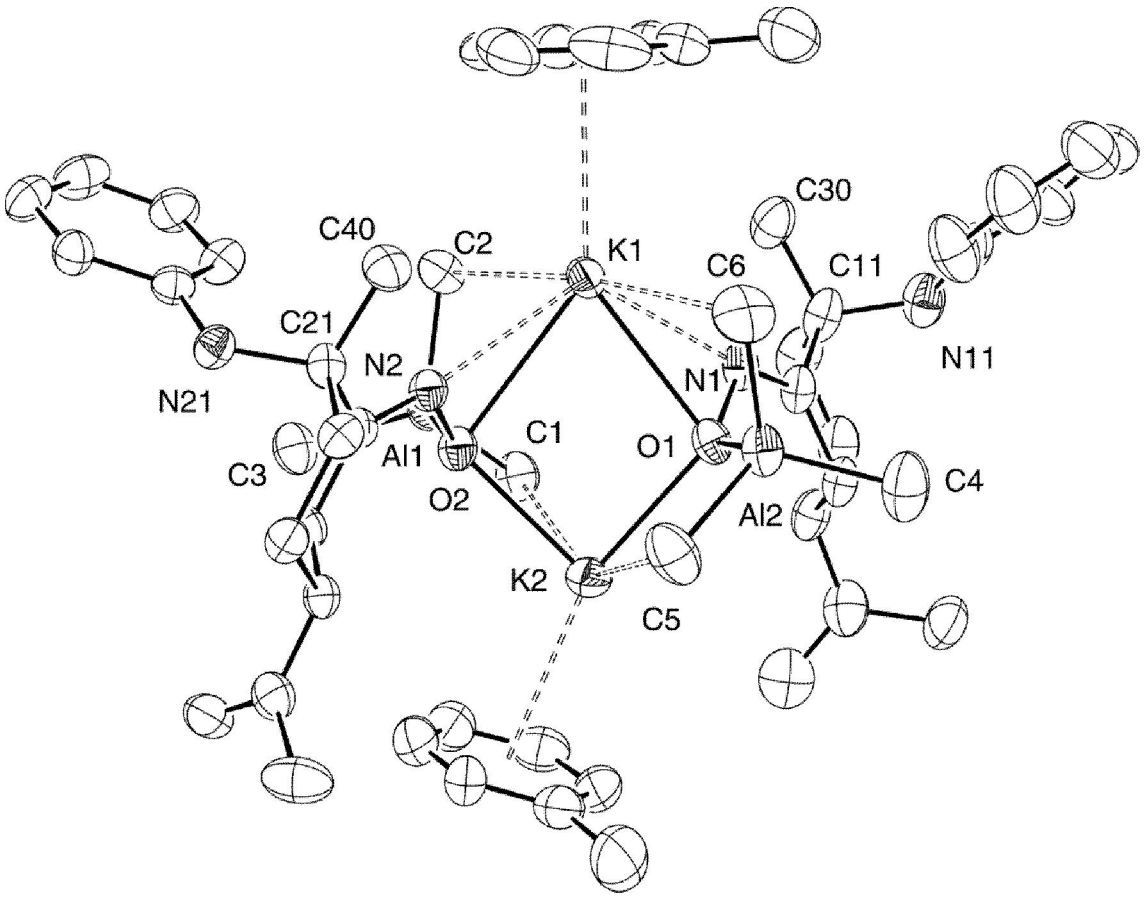


Figure S29a. Molecular structure of **(1*S*,4*R*)-1a**

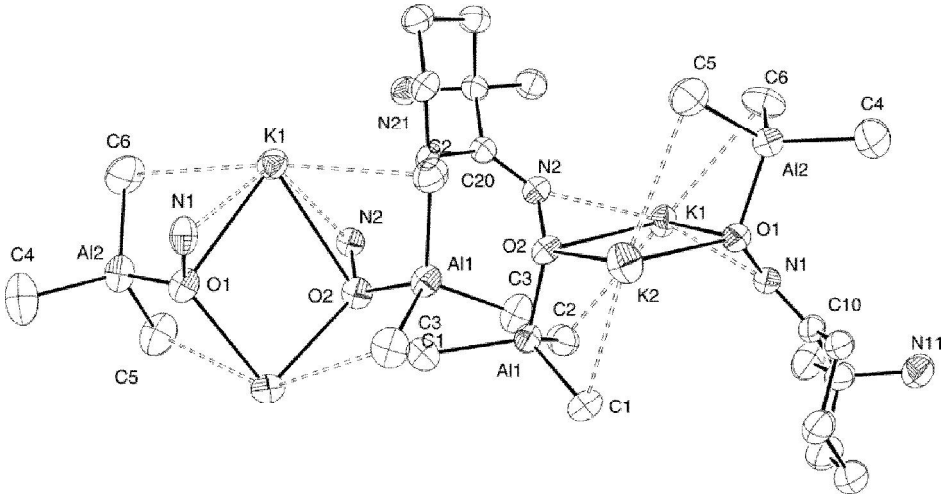


Figure S29b. Two views of **(1*S*,4*R*)-1a** core.

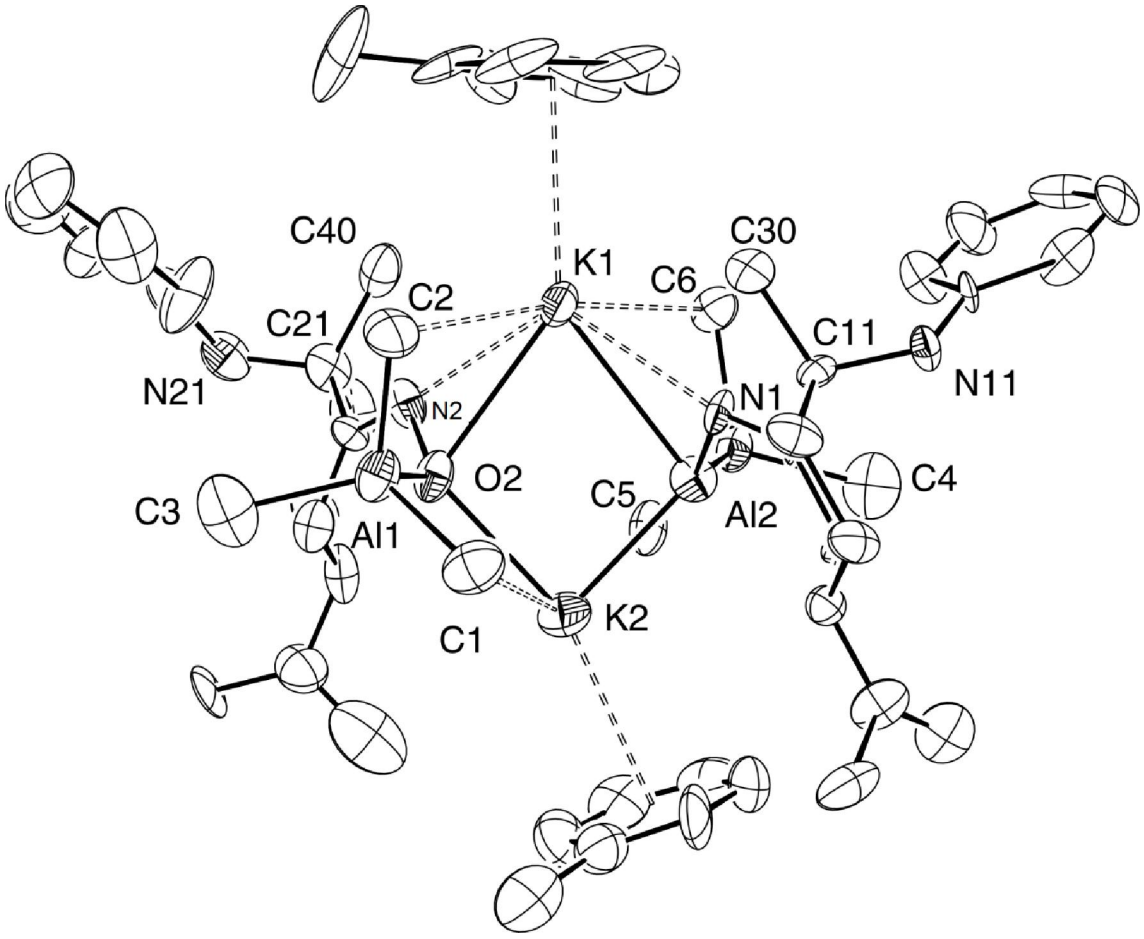


Figure S30a. Molecular structure of **(1*R*,4*S*)-1a·**

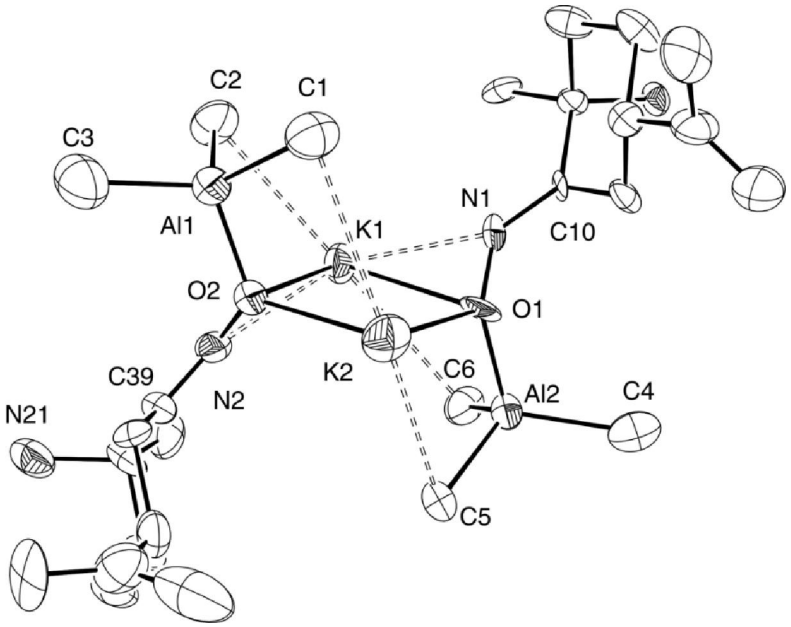


Figure S30b. (1*R*,4*S*)-1a·core

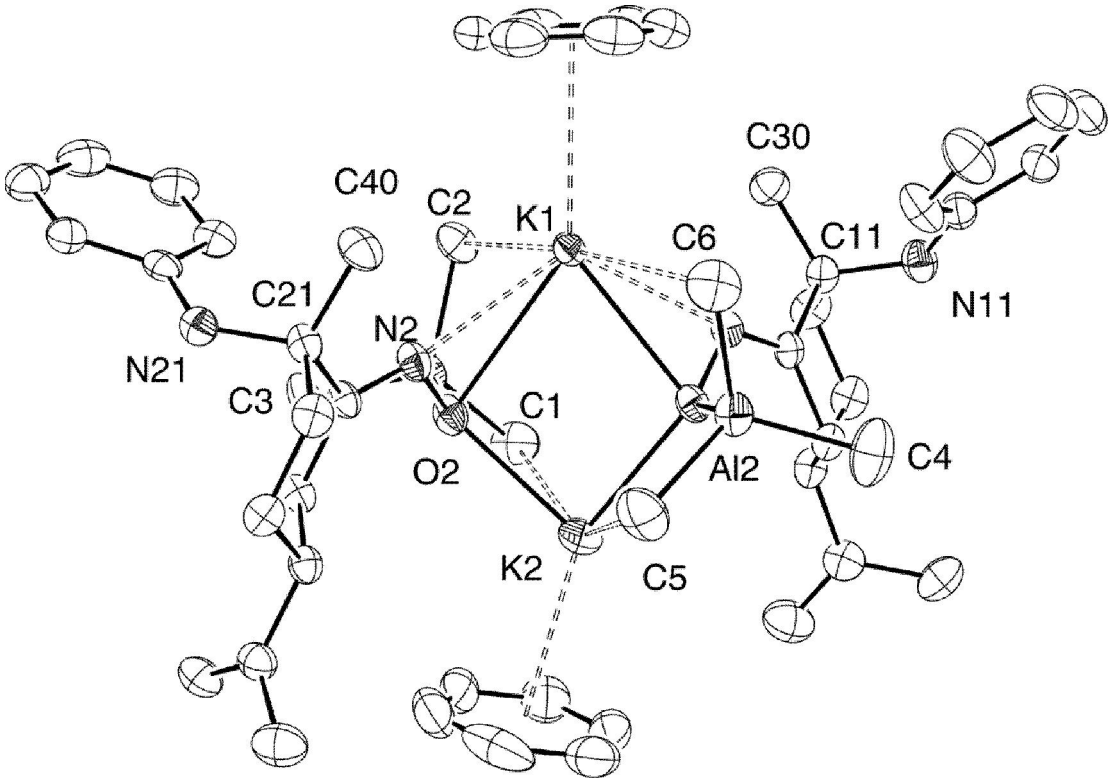


Figure S31a. Molecular structure of **(1*S*,4*R*)-1aC_6D_6**.

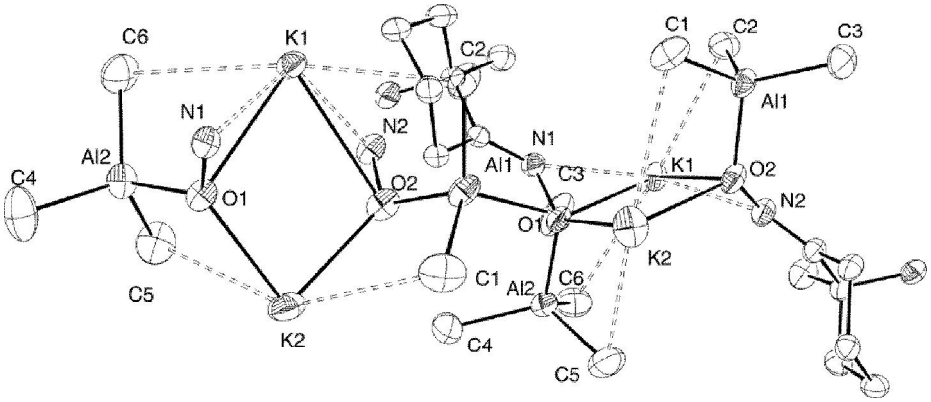


Figure S31b. Two views of **(1*S*,4*R*)-1a** core.

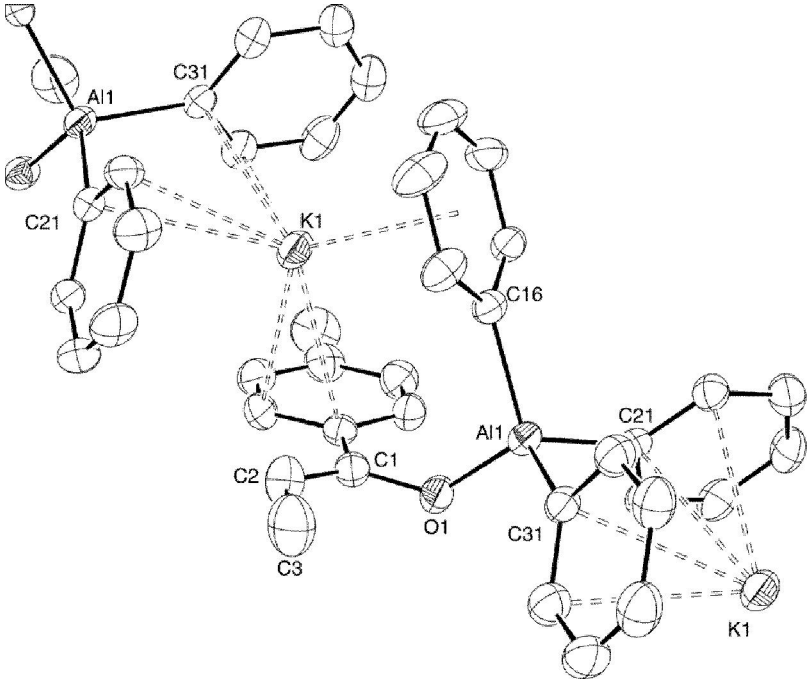


Figure S32. Molecular structure of **3**.

Table S4. Selected bond lengths [Å] and angles [deg] for **3·C_6H_6.**

BONDS (Å)		**ANGLES (º)**	
O(1)-C(1)#1	1.347(4)	C(1)#1-O(1)-Al(1)	130.8(2)
O(1)-Al(1)	1.753(3)	O(1)-Al(1)-C(31)	112.00(16)
Al(1)-C(31)	1.990(4)	O(1)-Al(1)-C(21)	108.31(15)
Al(1)-C(21)	1.998(4)	C(31)-Al(1)-C(21)	105.31(15)
Al(1)-C(16)#1	1.994(4)	O(1)-Al(1)-C(16)#1	109.77(13)
C(1)-C(2)	1.319(6)	C(31)-Al(1)-C(16)#1	111.71(16)
C(1)-O(1)#2	1.347(4)	C(21)-Al(1)-C(16)#1	109.57(17)
C(1)-C(10)	1.483(6)	C(2)-C(1)-O(1)#2	121.7(5)
C(2)-C(3)	1.491(7)	C(2)-C(1)-C(10)	123.0(4)
		O(1)#2-C(1)-C(10)	115.3(4)
		C(1)-C(2)-C(3)	125.2(5)

V. Computational Details.

Electronic structure calculations were carried out with the B3LYP[10] density functional along with the 6-31G(d) basis set. Minimum energy and transition state structures were optimized by computing analytical energy gradients. The obtained stationary points were characterized by performing energy second derivatives, confirming them as minima or first order saddle points by the number of negative eigenvalues of the hessian matrix of the energy (zero and one negative eigenvalues respectively). To further refine the energies obtained from the B3LYP/6-31G(d) calculations and to describe solvation effects, single-point calculations in toluene solution using the IEF-PCM model[11] on the previously optimized gas phase structures were performed using the larger 6-311+G(2d,p) basis set. In order to compare the reaction and activation energies obtained with the hybrid B3LYP functional, single point calculations with the pure BP86[12] and hybrid meta-GGA M06-2X[13] functionals and the 6-311+G(2d,p) basis set in toluene solution on the B3LYP/6-31G(d) optimized structures were also performed. Computed electronic energies were corrected for zero-point energy, thermal energy, and entropic effects to obtain the corresponding thermodynamic properties H^0 and G^0 at 298.15 K. All calculations were carried out with the Gaussian 09 suite of programs.[14]

A truncated model (**1c$_m$**) was used where the ONL_1 ligands and the ancillary ketone not converted to the enolate in **1c** were replaced by $ON{=}CMe_2$ and acetone respectively. The optimized geometry of the starting K-Al model complex is in reasonably good agreement with the structure determined by X-ray crystallography for **1c** (Table S5). The computed structure of **1c$_m$** is more symmetrical and has significantly longer K-C(benzene) distances than those found in the X-ray structure of **1c**. However, minimization of **1c$_m$** while constraining it to have the crystallographic K-C(benzene) metrics gave an energy that is only 1.6 kcal/mol higher.

Different functionals were employed to test the dependence of the energetic results obtained by DFT with the functional used. Several alternative mechanisms were

studied as shown in Figure S29. Although the relative values obtained with the three functionals are different (Table S6), independently of the computational method employed, the lowest energy path found yielding the enolate complex $\mathbf{2_m}$ is that shown in Scheme 3 in the main text of the current article.

Table S5. Comparison of selected bond lengths (Å) and angles (degrees) for the optimized structure of $\mathbf{1c_m}$ and the X-ray structure of **1c**.

	$\mathbf{1c_m}$ (calc)[a]	**1c** (expt)[a]
K1-O	2.916	2.931
K1-N	2.755	2.726
K1-C(benzene)	3.524	3.384
K2-O	2.633	2.566
K2-C(benzene)	3.494	3.226
Al-O	1.888	1.831
Al-CH_3	2.016	1.975
N-O	1.404	1.415
C=N	1.285	1.275
O1-K1-O2	78.0	74.1
O1-K2-O2	88.4	87.1
K2-O-K1	96.8	99.3
N-O-Al	116.6	117.5
N-O-K2	135.2	130.0
N-O-K1	69.1	67.6
Al-O-K2	107.2	111.3
Al-O-K1	98.4	97.4

[a] Average values

Table S6. Relative enthalpies and Gibbs energies (between brackets) at 298.15 K for all the species studied. All values in kcal/mol. Data in bold font correspond to the highest stationary point (both in *H* and *G*) along a certain mechanistic pathway (See Figure S32).

	B3LYP	BP86	M06-2x
$\mathbf{1c_m}$	0.0; [0.0]	0.0; [0.0]	0.0; [0.0]
$\mathbf{Ic_m}$	-6.7; [-8.7]	-5.6; [-7.5]	-0.3; [-2.2]
TS($\mathbf{Ic_m}$-$\mathbf{IIc_m}$)	**24.2; [29.7]**	**19.4; [24.8]**	19.8; [25.3]
$\mathbf{IIc_m}$	9.3; [15.1]	7.0; [12.7]	-1.5; [4.2]
TS($\mathbf{IIc_m}$-$\mathbf{IIIc_m}$)	20.5; [23.7]	15.7; [18.9]	**22.5; [25.7]**
$\mathbf{IIIc_m}$	6.0; [9.4]	4.9; [8.3]	0.9; [4.3]
TS($\mathbf{IIIc_m}$-$\mathbf{2_m}$)	20.8; [23.5]	16.2; [18.9]	19.0; [21.8]
$\mathbf{2_m}$	-32.7; [-39.3]	-31.1; [-37.7]	-29.8; [-36.4]
TS($\mathbf{Ic_m}$-$\mathbf{2_m}$)	**34.5; [38.7]**	**27.9; [32.1]**	**32.5; [36.8]**
TS($\mathbf{IIc_m}$-$\mathbf{2_m}$)	**46.9; [50.5]**	**38.2; [41.8]**	**50.1; [53.7]**
TS($\mathbf{IIc_m}$-$\mathbf{IVc_m}$)	21.5; [26.1]	14.4; [19.0]	23.2; [27.8]
$\mathbf{IVc_m}$	11.9; [16.0]	9.2; [13.3]	11.0; [15.2]
TS($\mathbf{IVc_m}$-$\mathbf{2_m}$)	**27.3; [31.3]**	**21.3; [25.3]**	**26.0; [30.0]**

Ic'$_m$	-7.9; [-7.5]	-6.8; [-6.4]	-2.7; [-2.3]
TS(Ic'$_m$-IIc'$_m$)	**28.8; [32.7]**	**25.6; [29.4]**	**28.7; [32.5]**
IIc'$_m$	18.4; [20.1]	17.1; [18.7]	25.6; [27.2]
TS(Ic'$_m$-2'$_m$)	**44.9; [50.0]**	**36.2; [41.3]**	**40.7; [45.7]**
2'$_m$	-31.9; [-39.2]	-30.3; [-37.5]	-28.7; [-36.0]
TS(Ic$_m$-Vc$_m$)	**26.1; [30.5]**	**21.0; [25.4]**	**26.1; [30.5]**
Vc$_m$	-30.9; [-26.0]	-30.0; [-25.1]	-39.9; [-35.0]
TS(Ic'$_m$-Vc'$_m$)	**26.0; [30.0]**	**20.6; [24.6]**	**26.2; [30.3]**
Vc'$_m$	-31.9; [-26.6]	-31.0; [-25.7]	-40.2; [-34.9]

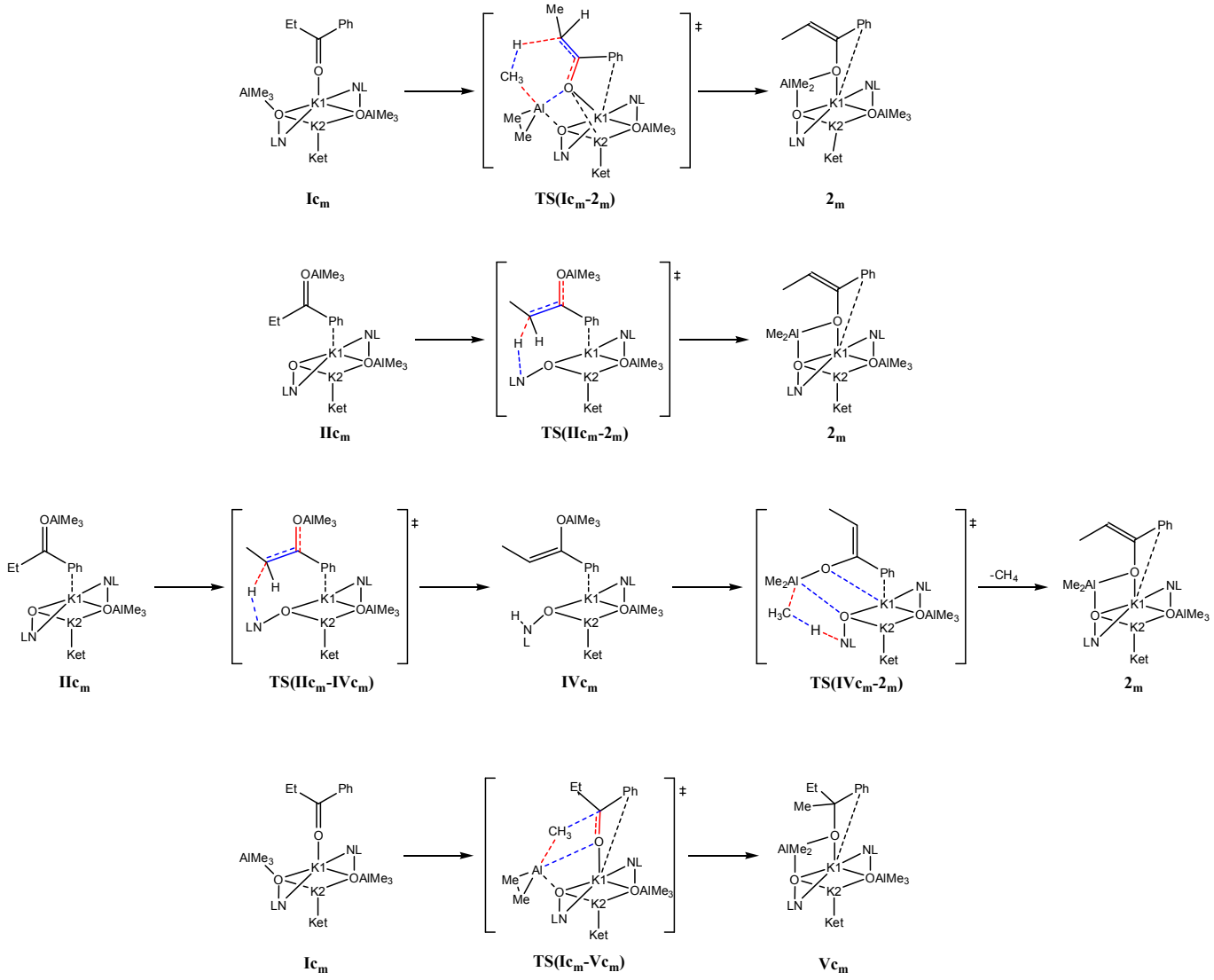


Figure S33. Alternative mechanisms computationally explored by DFT calculations. Ket = Me_2CO, L = CMe_2. Stereochemistry and formal charges not shown for simplicity. Bonds being broken and formed in the transition states in red and blue respectively. The analogous possible pathways where the ketone that converts to the enolate is the one coordinated to the K2 potassium were also studied (**Ic'$_m$** → **2'$_m$**; **IIc'$_m$** → **2'$_m$**; **Ic'$_m$** → **V'$_m$**)

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Cartesian Coordinates

1c$_m$				**Ic$_m$**			
C	-0.02850800	4.52101400	-1.68166200	C	-0.52070200	-4.68827300	1.18023900
C	-1.63764000	1.70438300	-2.60448800	C	-2.59071700	-2.27251700	2.29301100
C	1.66908200	1.75202100	-2.57472500	C	0.70116300	-1.90513000	2.62183000
C	1.08415800	-3.43522800	-2.95957900	C	-0.73689200	3.24488800	3.59039000
C	-5.35473000	1.27142300	-0.68463400	C	6.47034000	-2.18882000	0.58066900
C	5.25595300	0.23195000	-1.38811600	C	5.48167700	-1.21076200	0.58370100
C	-5.30916500	0.07494200	-1.40893300	C	7.76188900	-1.87586500	0.14565600
C	5.23543400	-1.12211700	-1.03686300	C	-1.50931100	2.77508000	2.38725500
C	5.27156700	1.21262900	-0.39046200	C	-3.01146800	2.90107900	2.39562800
C	0.12383800	-2.95888800	-1.90329400	C	8.06015700	-0.58125600	-0.28326100
C	-1.33577900	-3.30318600	-2.04997600	C	5.76959600	0.09756300	0.15627400
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C	5.22931000	-1.49559000	0.31138700	C	1.25583300	-2.59544800	-3.03151800
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H	-5.42142700	2.17112100	1.27629000	H	-1.83390500	5.14140300	-2.05790100
H	-5.26012200	-2.08052800	-1.29599100	N	-0.82978200	2.27736700	1.41665500
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H	5.28147200	1.60124700	1.73224100	Al	-0.77474600	-2.73332300	1.51267300
H	-5.37081900	-0.00832200	2.47515900	Al	-1.37707000	2.67621200	-1.31369800
H	5.23521600	-0.80657300	2.35536500	K	0.90761100	0.35951700	0.45327700
H	0.25347500	-4.96338300	1.12709600	K	-3.03368800	-0.35457800	-0.11870600
H	-1.47514100	-4.69329900	1.35499300	H	0.50060600	-0.87756100	2.96956200
H	-0.41535300	-4.85432500	2.75089400	H	0.82227700	-2.49879100	3.54059600
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Al	0.00045400	2.52427300	-1.73317900	H	1.27886700	2.82602000	-1.16902200
Al	-0.16526400	-2.44885000	1.76001600	H	0.82892900	1.43330100	-2.18866100
K	2.01705600	-0.07609600	-0.03159900	H	0.70828400	3.06737600	-2.80966300
K	-2.13094300	0.11988000	0.02731200	H	-2.73622300	-1.21243300	2.56434000
H	1.63716400	0.66206100	-2.74224700	H	-3.45347800	-2.58820900	1.68202500
H	1.78086000	2.19200200	-3.57748200	H	-2.69718400	-2.82188900	3.24070400
H	2.60713400	1.98889300	-2.04866000	C	4.67005600	1.10828900	0.17360900
H	-1.64399000	-1.72360900	3.74879200	C	4.92860800	2.53869400	-0.27137000
H	-1.44785400	-0.30457300	2.74904700	H	4.19252100	3.16667200	0.23950800
H	-2.64522100	-1.55922600	2.32628200	O	3.53457100	0.77895300	0.51525600
H	2.50276000	-2.26878800	1.91694700	C	4.76281700	2.69232600	-1.79808000
H	1.76430700	-0.84076700	2.68871500	H	4.94560200	3.73115200	-2.09099900
H	1.75023000	-2.39400900	3.49219100	H	5.46456900	2.05522300	-2.34732900
H	-1.61377300	0.60569500	-2.70937200	H	3.74461400	2.42989100	-2.10240900
H	-2.60291100	1.98231200	-2.14986900	H	5.92495800	2.87242000	0.03668700
H	-1.68937600	2.08394100	-3.63623800	O	-5.66672600	-0.64503100	-0.38590400
H	5.21293600	-2.54692900	0.58496700	C	-6.87822200	-0.74619400	-0.51958900
H	-5.29195700	-2.13149900	1.18940500	C	-7.65408100	-1.85510100	0.15714800
H	-1.88219400	-2.46579800	-2.50745000	C	-7.66092700	0.23251000	-1.36741600
H	-1.46719400	-4.17345500	-2.70060800	H	-8.28538300	0.85857600	-0.71646100
H	0.79732100	-3.05332000	-3.94868000	H	-8.34079900	-0.29435700	-2.04705400
H	1.07543300	-4.53107000	-3.02461100	H	0.33482500	3.07995400	3.45073900
H	2.10188800	-3.10421100	-2.73646600	H	-0.91012600	4.31425900	3.76890700
H	2.47258500	2.87523100	2.69303900	H	-3.47775400	1.93153100	2.62174800
H	1.60097900	4.38881800	3.04318600	H	2.12410800	-2.08300600	-2.60872900

H	1.21104000	2.92567400	3.95007500	H	-1.06174100	2.71267200	4.49475000
H	-1.57946900	2.61278900	2.52626700	H	1.00318700	-2.12860400	-3.99321200
				H	1.52862400	-3.63760500	-3.24355800
				H	-1.91407700	-2.41178600	-2.87230300
				H	-8.53541600	-1.45700300	0.67351200
				H	-8.02191800	-2.55768700	-0.60219300
				H	-7.01603800	-2.39112300	0.86241600
				H	-6.98282700	0.87238400	-1.93539500
TS(Ic_m-IIc_m)				**IIc_m**			
C	1.19260500	3.75087000	-3.48382600	C	-0.29933500	-3.55539400	-3.67782400
C	-4.89649100	1.84731600	-1.42258600	C	3.19714400	-1.10740300	-2.50410300
C	-4.01540400	0.76768200	-1.39993400	C	2.47979700	-0.08998100	-1.86775900
C	-5.83511700	2.00606800	-0.39872700	C	4.33834200	-1.64561400	-1.90267600
C	1.82784400	3.09956000	-2.28541600	C	-0.94064100	-2.80441700	-2.54176200
C	3.30161300	2.79022500	-2.32163200	C	-2.22071300	-2.05593000	-2.80949400
C	-5.89665000	1.07096700	0.63670800	C	4.76373200	-1.14280500	-0.66803600
C	-4.05742800	-0.17235700	-0.35215800	C	2.87761200	0.40160900	-0.61672600
C	0.24607600	-1.56040800	3.31609500	C	2.15468400	-0.72499400	4.35277700
C	-1.06828900	-1.07478100	2.76304700	C	1.49992100	0.14675600	3.31382000
C	-5.02131800	-0.01402600	0.65702100	C	4.04231400	-0.12630500	-0.03419300
C	-2.21528400	-0.85962500	3.71347200	C	0.42902600	1.10075700	3.76708600
C	-0.08440800	3.33133700	2.13217600	C	-0.14939700	-4.05610000	1.99117300
C	2.68073500	4.91016100	1.05271100	C	-3.03246500	-4.37380200	0.31720400
C	2.90834600	1.88838200	2.52492300	C	-2.40507400	-1.62291300	2.20656500
H	-4.86103400	2.55678600	-2.24500200	H	2.86835600	-1.47318800	-3.47326200
H	-3.30560800	0.61932400	-2.20904600	H	1.60176900	0.34489400	-2.33163600
H	-6.52133900	2.84815200	-0.41397500	H	4.90271400	-2.43145600	-2.39798400
H	3.77820700	3.07102000	-1.37901400	H	-2.88554500	-2.09546000	-1.94416800
H	3.45816700	1.71189700	-2.46062600	H	-2.00968000	-0.99851800	-3.02521700
H	0.72557600	-2.24370400	2.60883300	H	2.93500900	-1.34878100	3.90861300
H	0.10399400	-2.07272300	4.27379600	H	1.41160000	-1.37575300	4.83171800
H	-6.62777800	1.18679000	1.43174800	H	5.66489000	-1.53383800	-0.20192800
H	-5.07710200	-0.72657000	1.47309600	H	4.38607400	0.24706500	0.92346600
H	2.12808600	5.53082900	0.33223100	H	-2.60978900	-5.07040600	-0.42148400
H	3.70382900	4.80702200	0.66081400	H	-3.87631500	-3.86618900	-0.17362700
H	2.76375200	5.50631800	1.97368300	H	-3.46900900	-4.99610700	1.11238900
N	1.05999500	2.82896000	-1.29121700	N	-0.33779200	-2.84201400	-1.40762600
N	-1.26502300	-0.81630700	1.51170700	N	1.90785800	-0.00818100	2.10223000
O	-0.21487400	-0.95179500	0.66283200	O	1.17506300	0.75974700	1.16711200
O	1.69811300	2.17764300	-0.21994900	O	-0.94464400	-2.09048700	-0.38180600
Al	-0.32104000	-2.29120800	-1.28836600	Al	0.01191200	3.46232200	-1.02057500
Al	1.79801300	3.15121700	1.39521900	Al	-1.67701800	-3.10110700	1.04343700
K	-1.00210300	1.44883000	-0.15458500	K	1.66890300	-2.29699700	0.34526400
K	2.32800400	-0.37113400	0.38287400	K	-1.37547600	0.54580700	-0.03810200
H	3.21641800	2.41689600	3.43961600	H	-2.82382100	-2.05470100	3.12824900
H	2.39069400	0.98270400	2.88299900	H	-1.64182700	-0.90174100	2.54345000
H	3.84989200	1.57072200	2.04563900	H	-3.22442800	-1.04981500	1.74674800
H	-0.79338200	3.84884900	1.46323700	H	0.47962000	-4.69476300	1.34765600
H	-0.55048300	2.38685300	2.46096400	H	0.51663600	-3.41811800	2.59890600
H	-0.04129200	3.95787400	3.03588900	H	-0.60284600	-4.75067700	2.71412700
C	-3.08051600	-1.30335300	-0.36194100	C	2.01177400	1.47311600	0.07406100
C	-3.43514900	-2.61442600	0.30284800	C	2.83164600	2.54880300	0.80839300
H	-2.52375200	-3.20944800	0.39120100	H	2.10449500	3.24600000	1.23862400
H	-3.80413900	-2.43395100	1.31642000	H	3.36321000	2.08804900	1.64980100
O	-2.07217800	-1.18754500	-1.08423900	O	1.06556600	1.93499800	-0.75478800
C	-4.49595600	-3.38354700	-0.51276900	C	3.82540300	3.30508700	-0.08152800
H	-5.43119600	-2.81908600	-0.59236500	H	4.61616800	2.64613700	-0.45639500
H	-4.13144800	-3.59666700	-1.52173700	H	3.32375700	3.75723400	-0.94023000
H	-4.71619000	-4.33744700	-0.02259200	H	4.30413300	4.10876500	0.48915400
C	0.62034100	-3.62489000	-0.08943500	C	-0.84964300	3.94383400	0.74878200
H	0.94712100	-4.49332600	-0.68281400	H	-1.57683100	4.75585400	0.58487400
H	1.50700200	-3.23898200	0.43812000	H	-1.40639100	3.14500100	1.26871300
H	-0.03905800	-4.02217500	0.69767300	H	-0.12853300	4.33411100	1.48316900
C	-1.25250700	-3.46062400	-2.65202700	C	1.04467400	4.97518800	-1.81824800
H	-1.88451400	-2.91337700	-3.36827100	H	1.65064400	4.67399800	-2.68560700
H	-0.49886600	-3.99520000	-3.25278100	H	0.34701000	5.74297400	-2.18735800
H	-1.88448700	-4.24686500	-2.20914700	H	1.72056700	5.48837800	-1.11999400
C	0.84055700	-0.98058500	-2.31208400	C	-1.35044700	2.70620100	-2.32695700
H	0.94220100	0.05795600	-1.96425500	H	-0.96950100	1.83589900	-2.88804300
H	1.86469100	-1.37323500	-2.44049300	H	-2.32826900	2.42123000	-1.90502300
H	0.43512200	-0.91010300	-3.33206200	H	-1.57847900	3.46632300	-3.08905300
H	1.66567400	4.71909000	-3.69325500	H	-0.97684600	-4.33137500	-4.05698600
H	1.32380400	3.12956400	-4.38001100	H	-0.08447200	-2.88231200	-4.51891000
H	0.12372700	3.91146100	-3.31808100	H	0.63111600	-4.03000200	-3.35497500
H	3.79197800	3.31157700	-3.14922100	H	-2.73546900	-2.46796100	-3.68299000
H	-3.09131200	-0.47572700	3.18277400	H	0.27154100	1.89775400	3.03946400

H	-2.49074600	-1.79233400	4.22603400	H	-0.52011300	0.56446800	3.90123600
H	-1.94741500	-0.13774100	4.49762300	H	0.69439800	1.53050900	4.73919500
H	0.93270300	-0.72058900	3.49688700	H	2.59948100	-0.10920700	5.14430500
O	4.56708200	-1.80948000	0.17579500	O	-4.00600700	1.10436100	0.04268200
C	5.29183900	-2.76848100	-0.05408000	C	-5.03005400	1.76612400	0.13952400
C	4.73652400	-4.07546600	-0.57465100	C	-4.99024900	3.26870700	0.31117400
H	4.97607200	-4.16229100	-1.64327700	H	-3.97465800	3.60554500	0.52795700
H	5.20282900	-4.93170500	-0.07434400	H	-5.33127100	3.74515500	-0.61770000
H	3.65170600	-4.11143000	-0.45382500	H	-5.67514000	3.59152100	1.10402600
C	6.78701300	-2.68596700	0.16444400	C	-6.39262700	1.10900700	0.08644200
H	7.08366100	-1.65828300	0.38292300	H	-6.29649800	0.05727500	-0.18975900
H	7.06774000	-3.33034200	1.00790300	H	-6.87066200	1.18056600	1.07216600
H	7.32991400	-3.05807400	-0.71249500	H	-7.04836500	1.62770500	-0.62294900
TS($\mathbf{IIc_m}$-$\mathbf{IIIc_m}$)				**$\mathbf{IIIc_m}$**			
C	-2.73749800	-0.26101600	3.88819300	C	-0.42309700	-2.95079200	-3.76278100
C	-4.70101000	0.62581500	0.24278500	C	3.95921800	-1.28952300	-2.52028900
C	-3.47733500	1.23074900	-0.04365100	C	3.37017900	-0.18523100	-1.90091100
C	-5.28532300	-0.25066200	-0.67444200	C	5.02402800	-1.95840600	-1.90987200
C	-1.34958200	-0.45455700	3.33964100	C	-1.18811000	-2.33907800	-2.62026100
C	-0.19704100	0.21613100	4.04041900	C	-2.57728600	-1.81956100	-2.88099900
C	-4.64164600	-0.51132700	-1.88919900	C	5.49657600	-1.50782800	-0.67445600
C	-2.82099300	0.98072600	-1.26194800	C	3.83905800	0.28405600	-0.65824800
C	2.12363700	-2.13055800	-3.50345400	C	-0.20926200	0.74682000	4.65116300
C	0.69691800	-2.58557700	-3.34635500	C	0.73947600	-0.15474600	3.90850100
C	-3.42439600	0.10275200	-2.18466100	C	4.90775900	-0.40454300	-0.05395900
C	0.25282300	-3.84008900	-4.04790700	C	1.36469200	-1.30855600	4.64301800
C	-0.08570000	-4.34699500	0.92991600	C	-0.32908800	-3.71989100	1.70973500
C	1.03673900	-3.42726500	3.94176800	C	-3.24465300	-4.12516300	0.09814100
C	2.73068700	-2.56580700	1.15035500	C	-2.81796900	-1.49927900	2.15219600
H	-5.19653000	0.83818600	1.18588900	H	3.58771800	-1.62378900	-3.48582700
H	-3.01610900	1.90157700	0.67156600	H	2.54379100	0.32797800	-2.38308400
H	-6.23725100	-0.72404800	-0.44943400	H	5.47919900	-2.82015900	-2.39044000
H	0.65330400	-0.46485000	4.12255000	H	-3.23475500	-2.02315200	-2.03340000
H	0.13291100	1.09671200	3.47338500	H	-2.54218400	-0.73194300	-3.03253500
H	2.17578600	-1.04072600	-3.57041000	H	-0.15100000	1.76808300	4.26813400
H	2.58523800	-2.57947100	-4.38851700	H	0.00799900	0.73723900	5.72354700
H	-5.09116800	-1.18741200	-2.61165200	H	6.31911100	-2.02365300	-0.18522100
H	-2.93723700	-0.12514900	-3.12610800	H	5.26360400	-0.07969200	0.91957500
H	0.04820600	-3.48792500	4.42050000	H	-2.80981800	-4.73962900	-0.70378400
H	1.63132000	-2.71577000	4.53431800	H	-4.13965300	-3.64276000	-0.32331900
H	1.50691900	-4.41165700	4.08601700	H	-3.60900600	-4.83118500	0.85965500
N	-1.23426600	-1.17990300	2.28530200	N	-0.58589900	-2.27930000	-1.48690000
N	-0.17674100	-1.97521800	-2.62218600	N	1.05390300	-0.01601400	2.67104000
O	0.30129200	-0.85084900	-1.94675100	O	0.38196700	1.06408800	2.05114400
O	0.07896200	-1.28817100	1.78368500	O	-1.31493300	-1.65362400	-0.45282100
Al	-0.43623000	3.76950400	0.47433200	Al	0.83438400	2.68966900	-1.25066200
Al	0.93979500	-2.95881400	2.00121100	Al	-1.94961800	-2.82425300	0.88985900
K	-1.62266300	-2.01190500	-0.27736400	K	1.38082400	-1.51058000	0.23544900
K	1.53061800	0.23891000	0.14621900	K	-1.87827900	0.86123000	0.23934100
H	3.38901700	-3.43602000	1.29444000	H	-3.23573500	-2.04579400	3.01127100
H	2.70271200	-2.40165400	0.06062000	H	-2.13017000	-0.75574000	2.58668400
H	3.27040800	-1.71730300	1.60356700	H	-3.67117200	-0.95480400	1.71407800
H	-1.15509500	-4.43893000	1.18728900	H	0.32416700	-4.20337400	0.96416700
H	-0.00074200	-4.25803400	-0.16631800	H	0.29559100	-3.06584400	2.33948900
H	0.34410900	-5.33162100	1.16799100	H	-0.65734400	-4.53291400	2.37423000
C	-1.48968700	1.62342900	-1.50900100	C	3.17042400	1.43781100	0.01249100
C	-0.80138700	1.41900400	-2.73877900	C	3.86407000	2.32413400	0.75427700
H	-1.44619600	1.20068300	-3.59047500	H	4.94386300	2.20211000	0.79344900
O	-0.92309200	2.17680700	-0.50529500	O	1.81333600	1.48084900	-0.16201700
C	0.40098500	2.28266900	-3.09011200	C	3.28982600	3.49012000	1.50188600
H	0.10164700	3.28549000	-3.41778400	H	3.57825300	4.44475600	1.03994500
H	1.07232000	2.41328800	-2.23586200	H	2.19822800	3.45459700	1.53520800
H	0.97367300	1.81948100	-3.90097900	H	3.66300500	3.51476200	2.53499700
C	1.44455600	3.35638500	1.07343100	C	-0.40532200	3.67049100	0.02927700
H	1.85968100	4.25662100	1.55207800	H	-1.41152700	3.82011800	-0.39776800
H	1.51782000	2.56442000	1.83749300	H	-0.53628000	3.24516600	1.03701400
H	2.13763700	3.10956700	0.25425200	H	-0.00991800	4.68248000	0.20006700
C	-0.58941000	5.25244400	-0.84957100	C	2.10004700	3.87472900	-2.23258700
H	-1.57035000	5.27395400	-1.34674200	H	2.82686900	3.31892100	-2.84253600
H	-0.47450600	6.23045000	-0.35903300	H	1.55646000	4.53368500	-2.92684200
H	0.16943500	5.21048700	-1.64357500	H	2.68256000	4.53317100	-1.57352600
C	-1.71793700	3.83446400	2.01027200	C	-0.23661400	1.47465800	-2.47463000
H	-1.74328500	2.89950100	2.59085400	H	-0.41127700	0.44538100	-2.12693200
H	-1.42515300	4.62392600	2.71901700	H	-1.22147400	1.90741700	-2.71948300
H	-2.75416700	4.06055000	1.71896200	H	0.28341900	1.36741900	-3.43866300
H	-2.80101000	-0.63892700	4.91691700	H	-0.95499500	-3.82563600	-4.15850300

H	-2.99237300	0.80671400	3.92334900	H	-0.32401500	-2.23420200	-4.58906800
H	-3.47652700	-0.78384500	3.27504500	H	0.57457600	-3.26102300	-3.44084900
H	-0.49158800	0.55456500	5.03821500	H	-2.99758800	-2.26947700	-3.78586000
H	-0.79874200	-4.05175600	-3.83499800	H	2.04593000	-1.86773700	3.99680900
H	0.38248100	-3.74866500	-5.13456700	H	1.92090300	-0.94676700	5.51694200
H	0.85670000	-4.69979200	-3.72719400	H	0.59062400	-1.99380800	5.01116400
H	2.71612000	-2.42584300	-2.62685500	H	-1.24232000	0.39922800	4.51750800
O	4.07684700	0.88551300	-0.40759900	O	-4.34119800	1.71651000	-0.21881400
C	5.18178300	1.31532300	-0.10614400	C	-5.48883400	2.05357800	-0.47585300
C	6.40808800	0.95873600	-0.91728300	C	-6.66714400	1.18062400	-0.10428100
H	6.78635000	1.85604900	-1.42424800	H	-7.44444600	1.76676700	0.39970400
H	7.21303800	0.60015900	-0.26453200	H	-7.11977100	0.77303400	-1.01783600
H	6.16283900	0.19839800	-1.66112900	H	-6.34519000	0.35549600	0.53385800
C	5.37963200	2.21125400	1.09786400	C	-5.78546200	3.35947500	-1.17957200
H	6.10045400	3.00955500	0.88963900	H	-6.29968400	4.03879000	-0.48721000
H	4.42566700	2.63822300	1.41592600	H	-4.86039500	3.82761500	-1.52126500
H	5.79328800	1.61202500	1.92066600	H	-6.46218900	3.19991600	-2.02734700
H	-0.31499400	0.24002700	-2.41737000	H	0.98123600	1.29742700	1.28240900
TS(IIIc$_m$-2$_m$)				**2$_m$**			
C	-0.79974700	3.56616900	-2.79411900	C	0.37734400	2.33947300	-4.05212300
C	-4.82415200	-0.52443200	2.33757300	C	-6.02150200	0.77179000	-1.30933800
C	-4.10949700	-0.77046100	1.16340800	C	-4.99078900	-0.04424200	-1.77535900
C	-5.74695000	0.52102100	2.39518500	C	-6.12917200	1.06583700	0.05197200
C	0.37647700	2.97275400	-2.06728300	C	1.19411100	2.10576200	-2.81003300
C	1.72320400	2.96562200	-2.74550800	C	2.66990400	1.83380100	-2.95385700
C	-5.94264000	1.32232000	1.26696700	C	-5.19468000	0.53191000	0.94247300
C	-4.30384700	0.01977500	0.01471900	C	-4.04854200	-0.59958600	-0.89123100
C	1.97064900	-2.75202900	2.78657400	C	0.45223400	-1.32960900	4.16896900
C	0.77527200	-1.87630300	3.06016900	C	-0.62585000	-0.46568000	3.56819400
C	-5.22528000	1.08116400	0.09673600	C	-4.16455400	-0.28816400	0.47719800
C	0.45637500	-1.54305000	4.49301900	C	-1.48831900	0.35376600	4.48958100
C	0.47870800	2.81768000	2.65202700	C	-0.19353300	3.86443100	1.35865700
C	2.59169600	4.60452500	0.73610100	C	2.61242400	4.75664900	-0.27158600
C	3.44099500	1.52573000	1.78419900	C	2.68396900	2.37134200	2.11285500
H	-4.66102600	-1.15713300	3.20663200	H	-6.73606800	1.18970000	-2.01418100
H	-3.39783600	-1.58869700	1.12565500	H	-4.89838400	-0.24295200	-2.83908500
H	-6.30280700	0.71437700	3.30868500	H	-6.93015300	1.70495300	0.41390500
H	2.50066000	3.31540400	-2.06108300	H	3.03052000	2.15030700	-3.93740100
H	1.99441400	1.94736200	-3.05661600	H	3.23594100	2.35010400	-2.17491100
H	1.91861500	-3.17430100	1.78175200	H	0.56597900	-2.25622100	3.60175400
H	2.03239300	-3.56095800	3.52357400	H	0.22633200	-1.56210900	5.21423400
H	-6.64778600	2.14898100	1.30259300	H	-5.27235000	0.74549800	2.00606900
H	-5.36428900	1.73442500	-0.75931700	H	-3.44877300	-0.70676100	1.17872000
H	1.80551800	5.22507000	0.28137200	H	2.06764500	5.16086000	-1.13742400
H	3.42511500	4.57489200	0.01741800	H	3.59979000	4.43905900	-0.64042400
H	2.95897100	5.16697400	1.60756200	H	2.79596600	5.60833100	0.40019200
N	0.15722100	2.49440700	-0.89532900	N	0.57028200	2.14291600	-1.68760000
N	0.00865300	-1.36907100	2.15799300	N	-0.86026900	-0.36756400	2.30779900
O	0.36181900	-1.65121800	0.83044700	O	0.01583300	-1.10545800	1.49227500
O	1.27975200	1.90923700	-0.28087500	O	1.36264600	1.86484800	-0.55917000
Al	-1.54396800	-2.36897700	-1.56245800	Al	-0.71564400	-2.35114900	0.32934100
Al	1.93888600	2.78765700	1.25384400	Al	1.61614000	3.29386000	0.65383500
K	-1.13218500	0.79384200	0.84993700	K	-1.34471900	1.27083600	0.07193500
K	2.37384600	-0.46509800	-0.39379500	K	2.36441000	-0.28004900	0.57284800
H	3.99277500	1.98263900	2.61948200	H	2.93654800	3.12814500	2.87070100
H	3.12229300	0.53741200	2.15712800	H	2.13601000	1.58931500	2.66621800
H	4.19197300	1.36699000	0.99175200	H	3.65558200	1.95354300	1.79750500
H	-0.46120300	3.27863200	2.30580000	H	-0.92434800	4.12580600	0.57546600
H	0.23705100	1.83546900	3.09060200	H	-0.67084400	3.14805700	2.04833200
H	0.80757200	3.43856000	3.49893100	H	-0.06501100	4.78502900	1.94741900
C	-3.51634600	-0.25690800	-1.22430800	C	-2.93298500	-1.46948700	-1.37362800
C	-3.96386600	0.09331800	-2.44958600	C	-3.10600500	-2.31899600	-2.40858600
H	-4.96376000	0.51293200	-2.51671800	H	-4.10579100	-2.39556500	-2.82792800
O	-2.30764300	-0.83347400	-0.99498100	O	-1.76155700	-1.29132900	-0.71341500
C	-3.21486900	-0.06207600	-3.73909000	C	-2.04660300	-3.18911200	-3.01694800
H	-3.27939000	0.85588300	-4.33944600	H	-2.07364600	-3.13030500	-4.11382200
H	-2.15561200	-0.27681200	-3.56805300	H	-1.04745300	-2.89255700	-2.68711300
H	-3.62353800	-0.87232400	-4.35953700	H	-2.18329400	-4.24978300	-2.75867100
C	-1.30549600	-3.60077800	0.24571500	C	-1.76151800	-3.74492700	1.27507400
H	-2.39392100	-3.72766500	0.16750000	H	-2.50783200	-3.31932300	1.96077900
H	-0.83099200	-4.45768000	-0.25035200	H	-2.31140100	-4.39603900	0.58150900
H	-1.11232200	-3.73011900	1.31950500	H	-1.11747800	-4.40197900	1.87775500
C	-2.77544100	-3.53895400	-2.58405900	C	0.94447400	-2.94515800	-0.64245300
H	-2.86538100	-3.21802100	-3.63074000	H	0.74307400	-3.86206300	-1.21354500
H	-2.42363300	-4.58030200	-2.60591600	H	1.33200400	-2.21848300	-1.37553000
H	-3.79326300	-3.55600500	-2.17080200	H	1.76465500	-3.20046000	0.04842100

C	0.24562500	-2.00858700	-2.38573300
H	0.47628700	-0.93251400	-2.39553300
H	1.05887700	-2.54587700	-1.87580900
H	0.26611900	-2.33734500	-3.43371400
H	-0.61685700	4.62380500	-3.02545800
H	-0.96553600	3.05263400	-3.75064800
H	-1.70821500	3.48733200	-2.19157400
H	1.71498600	3.59693500	-3.63904200
H	-0.42319000	-0.89688200	4.55230000
H	0.26751800	-2.45568800	5.07364400
H	1.30171600	-1.02936500	4.97016900
H	2.89926800	-2.16979500	2.87686800
O	4.82722800	-1.33471800	-0.98071100
C	6.04357400	-1.44969300	-0.90704700
C	6.85548800	-0.65444500	0.09165200
H	7.47406400	-1.32323800	0.70252500
H	7.54526100	0.01384900	-0.43966100
H	6.20160500	-0.06207800	0.73511000
C	6.79465600	-2.39747400	-1.81653300
H	7.28001400	-3.17998100	-1.21945300
H	6.11114100	-2.85754700	-2.53267100
H	7.59251400	-1.86685600	-2.35014600
H	-0.50955400	-2.46763200	0.40666700
H	0.44331300	1.47772800	-4.73005000
H	0.75324000	3.21085500	-4.60394000
H	2.87448500	0.75786300	-2.85741000
H	-0.67273500	2.50831300	-3.79956000
H	-0.87345000	1.03506100	5.09254000
H	-2.03015200	-0.29448500	5.19053100
H	-2.21259800	0.94557000	3.92367100
H	1.41859400	-0.80583700	4.15128500
O	4.72191100	-1.39522700	0.02496600
C	5.54167000	-2.16938600	-0.45129400
C	7.02213500	-1.85962800	-0.41309200
H	7.58353200	-2.70178600	0.00872300
H	7.39428800	-1.71172600	-1.43514400
H	7.20599800	-0.95685600	0.17247500
C	5.11810900	-3.46917400	-1.09926800
H	4.02956700	-3.52955400	-1.16458400
H	5.56044700	-3.56507200	-2.09820000
H	5.49297800	-4.31420900	-0.50712600

TS(Ic_m-2_m)

C	3.81850000	3.28459600	2.14516500
C	2.84237100	0.06393800	2.37308900
C	0.69335300	2.53722500	3.12834000
C	-2.76926200	0.22352200	3.68896800
C	-3.95664500	2.98982900	-1.76866200
C	-2.89993900	2.10379400	-1.98896500
C	-5.18004600	2.51429900	-1.28817000
C	-1.75131100	-0.66117800	3.01348100
C	-0.77924300	-1.39558000	3.89363600
C	-5.33920700	1.14808500	-1.04359800
C	-3.04895000	0.72601500	-1.74758300
C	3.18480700	2.75779000	-1.86518700
C	1.94709200	3.44361000	-1.34691100
C	-4.28663700	0.26157700	-1.27654000
C	1.46072500	4.68551400	-2.04405600
C	-3.02147600	-3.49153500	-0.73050700
C	-2.08112300	-4.21336000	2.21816200
C	0.32779400	-4.00576200	-0.20011700
H	4.67723900	2.99843700	1.51876600
H	3.53135500	4.30152800	1.84015800
H	4.20306900	3.36851200	3.17269400
H	-3.82845100	4.04849500	-1.98160300
H	-1.94904400	2.46461800	-2.37315000
H	-6.00353200	3.20141100	-1.11263400
H	-0.35105300	-0.70467500	4.62919400
H	-1.29591400	-2.18683100	4.45076700
H	3.83505500	2.45929000	-1.03905900
H	3.73732600	3.41032300	-2.54821000
H	-6.28685400	0.77066000	-0.66763200
H	-4.41797300	-0.79606800	-1.07226500
H	-2.97870600	-3.72486800	2.62181100
H	-1.36558800	-4.29961000	3.04702100
H	-2.37508400	-5.23859200	1.95314700
N	-1.80858300	-0.70335700	1.72664400
N	1.25946300	3.03104800	-0.34344000
O	1.72965800	1.84132900	0.23966500
O	-0.85321700	-1.53049300	1.09807900
Al	2.30541100	1.98483100	2.02778100
Al	-1.28325400	-3.24380600	0.68040100
K	-1.01941200	1.81651100	0.55273100
K	1.37797700	-0.73547900	-0.42562500
H	-0.07887800	1.75829800	3.24180200
H	1.01585100	2.77429700	4.15319500
H	0.20106000	3.45284500	2.75999300
H	0.17806300	-5.07694500	-0.39755000
H	0.59842800	-3.55726800	-1.16452400
H	1.20765300	-3.94038100	0.45831000
H	-3.39620800	-3.71558300	-1.73621800
H	-2.77688400	-4.49794400	-0.35079400
H	-3.86615400	-3.11695100	-0.14090000
H	2.01119600	-0.65953300	2.38839400
H	3.59128600	-0.30237100	1.65128000

TS(IIc_m-2_m)

C	0.20652800	-3.99786800	-2.79347900
C	3.14455100	-3.10667500	0.13754900
C	3.23399800	-1.84377400	-0.44690800
C	3.41787500	-3.27178700	1.49988200
C	-0.85744500	-3.06302400	-2.28393600
C	-1.87474800	-2.52951400	-3.25920300
C	3.79288700	-2.16522000	2.26921700
C	3.61402900	-0.72332500	0.31661600
C	-0.21960900	3.03517600	3.07058600
C	0.41077400	1.69248300	3.32770500
C	3.90217400	-0.90560000	1.68178800
C	1.11329200	1.47420500	4.64092100
C	-2.31962800	-3.16588500	2.23154600
C	-4.14729900	-4.00139100	-0.45534400
C	-4.28151400	-0.87060100	0.79655200
H	2.86010600	-3.96198200	-0.46853300
H	3.01938700	-1.70671400	-1.50043200
H	3.35100200	-4.25631800	1.95536900
H	-1.88064700	-3.12099500	-4.17994400
H	-2.87361400	-2.53444100	-2.81701000
H	-0.85366200	2.97864200	2.18316200
H	0.53905400	3.81416600	2.90373100
H	4.01281000	-2.28570000	3.32623800
H	4.21464200	-0.06557900	2.29128000
H	-3.48746800	-4.82945600	-0.75402000
H	-4.65421200	-3.65702600	-1.36956500
H	-4.92878100	-4.44639400	0.17870000
N	-0.82494300	-2.76702000	-1.03323000
N	0.37827200	0.70141800	2.49555500
O	-0.24085800	0.86812700	1.30079000
O	-1.81546500	-1.86050600	-0.62048900
Al	2.23653100	1.84146500	-2.35974800
Al	-3.17243100	-2.54173500	0.50239000
K	0.25350300	-1.70275100	1.31910500
K	-1.91306100	0.78811000	-0.52377700
H	-5.20581100	-1.15239800	1.32316000
H	-3.80059600	-0.11094200	1.43461900
H	-4.61294600	-0.38057800	-0.13466900
H	-1.49466600	-3.88626000	2.09836300
H	-1.96766100	-2.35886600	2.89599600
H	-3.07730600	-3.70729500	2.81764500
C	3.73855600	0.59546600	-0.35439200
C	3.96806700	1.81330900	0.31770000
H	2.74049700	2.29180500	-0.16086100
H	4.00319500	1.76267600	1.40373400
O	3.44913700	0.63003000	-1.62304200
C	4.86298300	2.89667200	-0.27683000
H	5.87640600	2.81675400	0.13574500
H	4.93395600	2.80926000	-1.36310200
H	4.48837800	3.89958400	-0.04229800
C	1.53020300	2.93725200	-0.60358000
H	1.85551400	3.88570600	-0.15954100

H	3.31901600	-0.01848300	3.36145700	H	0.89866900	3.26838100	-1.45417800
C	-1.86280000	-0.17960400	-1.98858800	H	0.86405000	2.40709000	0.09168200
C	-2.10540100	-1.48735800	-2.48136000	C	3.06910000	3.08499200	-3.64814400
H	-2.35523500	-2.42198900	-1.30391700	H	3.77222100	3.80114700	-3.20579700
H	-3.09161500	-1.60492900	-2.93571500	H	3.61886000	2.53747800	-4.42651800
O	-0.71970500	0.29524800	-1.70455200	H	2.30217200	3.67483600	-4.17043400
C	-1.00667900	-2.22738600	-3.22245300	C	0.66108200	0.79094300	-2.97552700
H	-0.01749000	-1.96071600	-2.83812500	H	0.86439900	0.31172900	-3.94361600
H	-1.11502200	-3.31672200	-3.13183700	H	0.38997100	-0.01845500	-2.28300300
H	-1.00689300	-1.98921500	-4.29601600	H	-0.22627100	1.42371900	-3.13372300
H	2.22897500	5.46941000	-2.02029900	H	0.79884700	-3.52256300	-3.58721600
H	0.55479000	5.06850500	-1.56633900	H	-0.24662100	-4.89762900	-3.22965600
H	1.24605600	4.48052800	-3.10179100	H	-1.63385000	-1.49205300	-3.52866900
H	-3.44780000	0.66881500	2.95536300	H	0.87528100	-4.30156100	-1.98369000
H	0.02391400	-1.84445800	3.31072300	H	0.43272500	1.61733900	5.49341900
H	-3.36557200	-0.35913400	4.40300300	H	1.94167100	2.18513900	4.78322900
H	-2.27656100	1.02152100	4.25923000	H	1.51736500	0.45780600	4.69056800
H	2.91424400	1.84593600	-2.41485600	H	-0.81949600	3.35832100	3.93245700
O	3.61144000	-1.83571200	-1.41834100	O	-3.47255400	2.95837800	-0.81040700
C	4.71461000	-2.36155900	-1.46521300	C	-4.38739400	3.62480300	-0.34458600
C	5.74274900	-2.14485300	-0.37634000	C	-4.63549100	5.04300800	-0.81184300
H	6.19096200	-3.09579400	-0.06552000	H	-4.72848000	5.72262300	0.04361300
H	6.55836200	-1.52215800	-0.76728300	H	-3.82741800	5.37381300	-1.46716500
H	5.29243700	-1.64341700	0.48273400	H	-5.58694100	5.08828200	-1.35758000
C	5.10628700	-3.25763500	-2.62049900	C	-5.30864400	3.07551500	0.72252200
H	4.36095200	-3.19870700	-3.41603000	H	-6.35523600	3.31400500	0.50092200
H	6.09571300	-2.98859000	-3.00834900	H	-5.18262700	1.99525500	0.82661900
H	5.17374700	-4.29516700	-2.26758200	H	-5.06992100	3.55533900	1.68142800
TS(IIc_m-IVc_m)				**IVc_m**			
C	0.46977000	3.97383400	-3.03709600	C	1.50048500	3.34399500	-3.45518100
C	-3.63428800	2.53113400	-1.36909600	C	-3.27019500	2.64602200	-1.98164800
C	-3.32954100	1.16907300	-1.39707200	C	-3.10197300	1.26226700	-1.88469400
C	-4.19072600	3.10599800	-0.22221700	C	-3.86305600	3.36256200	-0.93645300
C	1.25213700	3.03788000	-2.15553600	C	1.97818400	2.48685400	-2.31389200
C	2.49894500	2.40191700	-2.71050800	C	3.18359000	1.61066800	-2.52900900
C	-4.44658900	2.30124900	0.89462600	C	-4.29292000	2.67300000	0.20381200
C	-3.57759800	0.34959700	-0.28109400	C	-3.53886800	0.55331500	-0.74985400
C	0.34716300	-1.29332700	3.97361400	C	-0.75797300	-0.62904400	4.38719700
C	-0.92600300	-1.80379200	3.35987100	C	-1.80944200	-1.13981200	3.45648100
C	-4.14761600	0.93797800	0.86449000	C	-4.13336100	1.28811800	0.29409800
C	-1.72853400	-2.85620400	4.07169500	C	-2.92299600	-2.02691500	3.92114000
C	1.15346600	3.32696900	2.61585000	C	1.06183200	3.66513300	2.18992300
C	3.74145100	4.02263400	0.61115100	C	4.09674600	3.58941000	0.77373600
C	3.40547900	0.93689800	1.92543400	C	2.92421300	0.90246800	2.46074500
H	-3.43732400	3.14382000	-2.24463800	H	-2.93853100	3.16542900	-2.87731100
H	-2.89000700	0.71932200	-2.28018600	H	-2.63182700	0.70328600	-2.68603100
H	-4.43210000	4.16528100	-0.20030300	H	-3.99621300	4.43859600	-1.01058100
H	3.27003500	2.32218000	-1.94174000	H	3.79231300	1.55760500	-1.62407500
H	2.27123200	1.38866600	-3.06860500	H	2.86056800	0.59144700	-2.78215100
H	1.21191800	-1.88333800	3.63527600	H	0.20742900	-1.11167900	4.18444400
H	0.31269700	-1.36589500	5.06588100	H	-1.03058000	-0.82142000	5.42778600
H	-4.88753100	2.73464700	1.78871300	H	-4.75600000	3.21461900	1.02510900
H	-4.34570900	0.33855500	1.74625300	H	-4.46459300	0.77918700	1.19449200
H	3.22717200	4.86247400	0.12128000	H	3.85239600	4.38222600	0.05154400
H	4.48126100	3.64290000	-0.10953300	H	4.88712200	2.97716500	0.31365400
H	4.31808400	4.45792000	1.44108600	H	4.56074000	4.09169100	1.63580400
N	0.78622700	2.82534700	-0.97689900	N	1.30188400	2.54539100	-1.22273900
N	-1.34722100	-1.37186800	2.21592800	N	-1.74117200	-0.81186400	2.20145700
O	-0.69794400	-0.46564800	1.50582500	O	-0.81229300	-0.06254000	1.66576800
O	1.51971300	1.90350200	-0.20351100	O	1.74720000	1.68807900	-0.19666200
Al	-1.13999900	-2.33347700	-2.30632300	Al	-1.03452400	-2.56987400	-1.86006600
Al	2.48662300	2.60847700	1.25939400	Al	2.50100000	2.51955400	1.32399900
K	-1.00767500	2.03910100	0.89528600	K	-0.89898400	2.23337300	0.33102500
K	1.42393900	-0.78513100	-0.12565100	K	1.42117300	-0.92690700	0.25235800
H	4.10357900	1.19665600	2.73569900	H	3.42774100	1.22549500	3.38454400
H	2.73693800	0.16937100	2.34737600	H	2.03424400	0.34216000	2.79025400
H	4.01548000	0.45706400	1.14365200	H	3.61429200	0.18972700	1.98089100
H	0.46988800	4.10189400	2.22790100	H	0.59312400	4.40382900	1.51740100
H	0.54919700	2.56685800	3.14084800	H	0.25749800	3.10789500	2.70154200
H	1.72444400	3.83032300	3.41039600	H	1.53544700	4.26582000	2.98091000
C	-3.20130600	-1.10303400	-0.35735700	C	-3.32475000	-0.93603800	-0.70819900
C	-3.51846500	-1.99156800	0.70516300	C	-4.10239900	-1.72145600	0.09740400
H	-2.48260500	-1.74250800	1.53473100	H	-2.47139700	-1.15249100	1.54141300
H	-4.36510300	-1.66515400	1.31204200	H	-4.90228200	-1.23468800	0.65030600
O	-2.55270400	-1.45282400	-1.39934500	O	-2.38878000	-1.35688000	-1.52977100
C	-3.50118000	-3.49202200	0.44677700	C	-4.10887000	-3.22513600	0.09136300

H	-4.28201900	-3.79015500	-0.26488600	H	-5.12071700	-3.60554500	-0.10497700
H	-2.54225200	-3.82232100	0.04235900	H	-3.44791800	-3.62320500	-0.68121400
H	-3.67758900	-4.04130300	1.37873200	H	-3.79350800	-3.66520800	1.05003300
C	-0.10183900	-3.45277800	-0.97750500	C	-0.44494000	-3.42990700	-0.10868400
H	0.96120800	-3.52068300	-1.26250100	H	0.59483600	-3.79294100	-0.17928300
H	-0.14238800	-3.12756400	0.07353800	H	-0.51645700	-2.82641800	0.81023500
H	-0.47144300	-4.48838900	-0.98070800	H	-1.05203400	-4.32599700	0.08390800
C	-2.01829700	-3.38642500	-3.74787500	C	-1.66323300	-3.93985000	-3.17005400
H	-2.64439800	-2.76671900	-4.40546900	H	-2.04520400	-3.48524200	-4.09567600
H	-1.27446500	-3.87311200	-4.39676000	H	-0.84126100	-4.60809400	-3.47119600
H	-2.66277900	-4.18769800	-3.35942400	H	-2.46313300	-4.59018400	-2.78739300
C	-0.05258100	-0.76813500	-2.98805500	C	0.41645500	-1.39413300	-2.66023600
H	-0.03932900	0.12829500	-2.34773600	H	0.46125100	-0.35991500	-2.28159500
H	0.99626800	-1.04032300	-3.19444500	H	1.43080400	-1.82248700	-2.58588900
H	-0.46388500	-0.42943100	-3.95069100	H	0.22084800	-1.29396900	-3.73836600
H	1.08715500	4.83220300	-3.33211600	H	2.28352000	4.04957100	-3.76171900
H	0.16184900	3.46802700	-3.96199700	H	1.26487500	2.72573700	-4.33172200
H	-0.42057700	4.34249200	-2.52036400	H	0.60935000	3.91001800	-3.17056600
H	2.88425700	2.97692600	-3.55823400	H	3.79206900	1.98376500	-3.35886900
H	-2.60839300	-3.15081900	3.49327700	H	-3.59611300	-2.30320200	3.10446600
H	-1.12247300	-3.75477300	4.25163000	H	-2.51934100	-2.94875400	4.35932300
H	-2.06258100	-2.49955500	5.05558900	H	-3.50951400	-1.53115900	4.70515800
H	0.52987400	-0.25653300	3.67905300	H	-0.59874500	0.44424000	4.23684300
O	3.65638800	-2.20524900	-0.51124700	O	3.66539700	-2.36242500	0.15168200
C	4.75921700	-2.72331500	-0.40565200	C	4.75483700	-2.90805500	0.04849200
C	5.64019500	-2.46766100	0.79809500	C	5.94042600	-2.46145900	0.87620700
H	5.66881000	-3.37167500	1.42141700	H	6.43982900	-3.31989900	1.34051300
H	6.67255300	-2.26074000	0.49324100	H	6.67921800	-1.98024400	0.22182900
H	5.24882000	-1.63663900	1.38863800	H	5.62491500	-1.74938800	1.64120400
C	5.29459300	-3.65037800	-1.47516000	C	4.97158300	-4.05528800	-0.91433500
H	5.68833400	-4.57233900	-1.03135600	H	5.14671700	-4.97960900	-0.34838100
H	4.51282200	-3.88629900	-2.19972600	H	4.09654600	-4.18600900	-1.55379800
H	6.13215500	-3.16405700	-1.99242600	H	5.86445700	-3.88531700	-1.52752800
TS(IVc$_m$-2$_m$)				**Ic'$_m$**			
C	-1.00670100	4.28903700	-2.05210200	C	0.88410400	-4.97258300	0.09507800
C	-4.48824500	2.30821700	-0.90583300	C	-1.31662900	-2.61127700	1.06604200
C	-3.89010400	1.04720700	-0.87951700	C	1.77363700	-2.59526400	2.30095200
C	-5.39145900	2.68172200	0.09097900	C	0.52911800	2.70995400	3.68194800
C	0.24423100	3.62641900	-1.54224000	C	0.08664200	2.49256800	2.26008300
C	1.55156000	3.90206200	-2.24013400	C	-1.29589000	2.93296000	1.85128400
C	-5.68962700	1.78090200	1.11615000	C	7.52322500	-0.05475400	2.23012400
C	-4.19454000	0.12154900	0.13536900	C	1.20870800	-2.83548500	-3.27499000
C	1.09133000	-2.33352000	3.22812200	C	2.38592300	-2.37073500	-2.45651500
C	0.42855900	-3.06594900	2.09471900	C	3.75142500	-2.37499800	-3.08921900
C	-5.09479000	0.52013100	1.14129600	C	3.20714900	2.38855200	-1.25224000
C	-0.08910300	-4.46109900	2.30830400	C	0.75122500	4.65226200	-0.96800300
C	0.74036600	2.40850700	3.00308800	C	0.32269200	1.89147600	-2.84856500
C	2.49108000	4.77594000	1.39716800	H	0.68333600	-5.69493900	0.90033400
C	3.70234400	1.64742100	1.63494600	H	0.21975800	-5.24896500	-0.73789400
H	-4.25132800	2.99750500	-1.71227200	H	1.91193500	-5.16875800	-0.24419300
H	-3.19035800	0.76521500	-1.66027900	H	-1.75391800	3.55447400	2.62662200
H	-5.85337900	3.66507800	0.07295700	H	-1.25653900	3.49220700	0.91260600
H	2.30885400	4.22675400	-1.52099400	H	0.52789800	-3.43490100	-2.66592100
H	1.93250400	2.99163000	-2.72085800	H	1.54047100	-3.42263300	-4.13681400
H	1.34270800	-3.01555600	4.04636600	H	1.10134700	5.05529400	-0.00604400
H	0.43714700	-1.54845500	3.63350500	H	-0.33073000	4.84959200	-1.01722400
H	-6.38048000	2.06431500	1.90620300	H	1.21084000	5.27907800	-1.74700900
H	-5.31610800	-0.16254200	1.95647700	N	0.92734300	1.93058500	1.46717100
H	1.61906100	5.39640500	1.14263200	N	2.30748700	-1.95547100	-1.24304400
H	3.26821900	5.00070400	0.65086300	O	1.00581100	-1.91642400	-0.71592200
H	2.86926000	5.16065500	2.35627700	O	0.44655800	1.70484600	0.16600600
N	0.12204100	2.85197300	-0.52395900	Al	0.62427700	-3.08873000	0.71041200
N	0.29905700	-2.51351700	0.93144500	Al	1.21170800	2.72209000	-1.22584000
O	0.75737300	-1.28159900	0.71613700	K	2.68827100	-0.05978100	0.72053400
O	1.31761500	2.23656800	-0.11185700	K	-0.98539900	-0.20037800	-0.95538100
Al	-1.56098100	-2.01619000	-1.81030700	H	1.53554000	-1.62428500	2.76806900
Al	2.05586300	2.82825600	1.52237500	H	1.60175600	-3.34040000	3.09253000
K	-0.91294800	0.74851400	0.93508100	H	2.85894900	-2.62322600	2.11140200
K	2.45960400	-0.05625400	-0.71449900	H	0.64406200	2.45682600	-3.73644400
H	4.32562800	2.00323600	2.46909300	H	0.61585500	0.84786200	-3.05501600
H	3.50026100	0.58572900	1.85287600	H	-0.77911200	1.94677600	-2.86108900
H	4.34980800	1.70113900	0.74317500	H	3.69491100	2.57686300	-0.28268700
H	-0.26081000	2.84608500	2.85210900	H	3.50174200	1.38329700	-1.59554300
H	0.61839000	1.33435400	3.22220500	H	3.67231700	3.08987200	-1.96148100
H	1.10713200	2.85203600	3.94085500	H	-1.48122900	-1.60609000	1.49049800
C	-3.55552900	-1.22919200	0.13989800	H	-1.97934100	-2.72669900	0.19184300

C	-4.19631500	-2.30816300	0.63633100	H	-1.70754100	-3.30993400	1.82128700
H	-0.18987100	-3.06154000	-0.25591400	C	6.44469800	0.40953200	1.27385600
H	-5.22270900	-2.16713300	0.96392000	C	6.87876600	1.25741300	0.09737800
O	-2.28822900	-1.24313700	-0.35518600	H	6.01075900	1.68018100	-0.41365700
C	-3.63628200	-3.69302300	0.75392300	O	5.27337800	0.10571800	1.44912200
H	-4.06678700	-4.37704400	0.00813600	H	7.55379300	2.05852600	0.42056800
H	-2.55168100	-3.69496400	0.62574000	O	-3.61002400	0.19817400	-0.99410100
H	-3.86147000	-4.12239000	1.73962800	C	-4.79339400	0.50620400	-0.85766200
C	-0.28949700	-3.82757500	-1.36887300	C	-5.63095700	-0.14797300	0.19058300
H	0.76550900	-4.10799700	-1.24132500	C	-5.41701500	1.56274100	-1.75995300
H	-0.90391600	-4.69296000	-1.09616000	C	-6.97540200	0.20339200	0.40199800
H	-0.37857400	-3.72679300	-2.46252900	C	-5.05183800	-1.14690400	0.99284000
C	-2.94600500	-2.88776200	-2.92796000	H	-5.80769200	2.36642600	-1.11971200
H	-3.77533700	-2.20042900	-3.14603000	H	-6.29991400	1.12095600	-2.24266100
H	-2.54470600	-3.21329500	-3.89845800	C	-4.45814300	2.12859100	-2.80589400
H	-3.39120200	-3.77267800	-2.45478300	C	-7.72181500	-0.42870900	1.39432900
C	-0.28916300	-0.75382300	-2.69860400	H	-7.44521000	0.97133400	-0.20381200
H	-0.15776600	0.19256300	-2.15516800	C	-5.80009800	-1.77774300	1.98188200
H	0.70386800	-1.20691800	-2.84464200	H	-4.01522000	-1.42404100	0.83165500
H	-0.64955100	-0.48320800	-3.70155600	H	-4.08683200	1.34186000	-3.46976600
H	-0.90469800	5.38169800	-2.01630200	H	-4.96890800	2.87875600	-3.41793200
H	-1.19087500	4.02029100	-3.10121900	H	-3.59140400	2.60405300	-2.33727400
H	-1.87243200	3.99651900	-1.45249600	C	-7.13581900	-1.41957500	2.18508600
H	1.43164500	4.66995900	-3.00993600	H	-8.75973900	-0.14867900	1.55035300
H	-0.51837000	-4.87849700	1.39413400	H	-5.34155100	-2.54942200	2.59353100
H	0.71494100	-5.12923900	2.64694600	H	-7.71952700	-1.91233000	2.95799100
H	-0.86341000	-4.48150500	3.08785800	H	1.54662700	2.33941000	3.83267800
H	1.99709100	-1.82595300	2.87935800	H	0.49999500	3.77738200	3.93725600
O	4.81208800	-1.21179800	-1.27119700	H	-1.94665800	2.06373600	1.68622100
C	5.93268500	-1.54439500	-0.90759700	H	4.50331600	-2.00183600	-2.38874700
C	6.81401200	-2.40509200	-1.78671900	H	-0.14224300	2.19520400	4.38255300
H	7.68025600	-1.82033700	-2.12251500	H	3.76530500	-1.74774000	-3.99083100
H	7.20817700	-3.25935300	-1.22356700	H	4.03069100	-3.39005000	-3.40074100
H	6.25588800	-2.75561000	-2.65703300	H	0.64399200	-1.97439200	-3.65985400
C	6.49166400	-1.12072800	0.43287600	H	7.11320100	-0.77212500	2.94362200
H	7.51267600	-0.73591500	0.32697100	H	7.44397000	0.63338300	-0.60796000
H	5.85365200	-0.36621000	0.89887600	H	8.36122600	-0.50369100	1.68380700
H	6.55192800	-1.99737300	1.09184500	H	7.92588200	0.80893900	2.77526600
TS(Ic'_m-IIc'_m)				**IIc'_m**			
C	-2.65825600	5.04453600	1.31012600	C	-2.88532100	4.14291800	2.52957800
C	-0.05845800	3.23324800	2.42921200	C	-0.39542300	1.89791700	2.88111600
C	-3.10762400	1.87631400	2.37823800	C	-3.51360400	0.83971000	2.43723500
C	-1.15883900	-2.85959200	3.44598800	C	-1.27062900	-3.91472400	-2.93937400
C	4.32900500	0.16648400	-0.07253000	C	3.26953500	-1.34534300	1.47702600
C	4.12125200	1.28714800	-0.90030800	C	2.84735300	-0.38209600	2.41571400
C	-0.25092000	-2.18600900	2.45201600	C	-0.54800700	-2.90341500	-2.09140800
C	1.22073100	-2.14521500	2.76341900	C	0.95342100	-2.96227700	-1.98647400
C	5.29533700	0.23997400	0.94464400	C	3.24330600	-2.70635200	1.83722800
C	4.85522800	2.45452400	-0.70616600	C	2.40000300	-0.76966800	3.67354600
C	6.01583500	1.41658200	1.14711500	C	2.78926100	-3.09068900	3.09563800
C	-1.39607200	4.25832800	-2.31408800	C	-1.54990600	4.62156500	-1.14191900
C	5.79798300	2.52380900	0.32493100	C	2.36631400	-2.12584700	4.01319600
C	-2.42657900	3.17602400	-2.11694000	C	-2.65114500	3.61788800	-1.36873300
C	-3.50655800	2.99974900	-3.14972000	C	-3.69096400	3.90102600	-2.41926200
C	-0.54490600	-0.94902900	-2.51494900	C	2.41473600	2.78366700	-1.69162200
C	0.39683800	-3.87247700	-0.77151000	C	4.43550100	0.65957900	-3.28537600
C	2.20509600	-2.49367200	-3.09381500	C	5.58426400	2.40950700	-0.57914600
H	-3.53439100	5.06084500	0.64524000	H	-3.75593700	4.44242300	1.92752000
H	-2.99972200	5.44415800	2.27662000	H	-3.20797400	4.19091800	3.58040700
H	-1.94328800	5.77957800	0.90989700	H	-2.12797800	4.93158900	2.40452800
H	3.40982200	1.21239500	-1.71836000	H	2.89649700	0.67016000	2.15593100
H	5.47130000	-0.61196000	1.59370800	H	3.55629400	-3.46901600	1.13302600
H	1.64112800	-3.15924800	2.81706900	H	1.34698900	-3.90395800	-2.38565700
H	4.70152400	3.30648900	-1.36250800	H	2.07048400	-0.01672400	4.38219300
H	1.74054500	-1.58655500	1.98400000	H	1.42391400	-2.13538600	-2.53877300
H	-0.39530300	3.82282500	-2.42929000	H	-1.52246000	4.92689200	-0.09125100
H	-1.35979100	4.91536900	-1.43983200	H	-1.69053500	5.50696200	-1.76894400
H	6.74883700	1.46803600	1.94682700	H	2.76101300	-4.14363400	3.35936400
H	-0.58453000	-3.86178400	-0.28293900	H	3.63184800	-0.02617700	-3.59144300
H	1.11614200	-4.17751000	0.00330900	H	5.37489300	0.08970900	-3.29519400
H	0.39487600	-4.67737800	-1.52154900	H	4.52229200	1.39676400	-4.09804100
N	-0.79039900	-1.67667300	1.39460600	N	-1.24729200	-1.99709300	-1.48553000
N	-2.44618200	2.37788400	-1.11047500	N	-2.76756500	2.51752400	-0.71498300
O	-1.39099300	2.56308300	-0.19923800	O	-1.74651400	2.28930100	0.22294600
O	0.01546500	-1.03802300	0.49091500	O	-0.57342500	-1.07674000	-0.76277800
Al	-1.87321000	3.21705600	1.50573100	Al	-2.19827500	2.32948400	2.04743500

Al	0.83422300	-2.12771300	-1.63897300	Al	4.05344000	1.63671600	-1.59104000
K	-2.55823700	-0.15632300	-0.00837900	K	-3.05901600	-0.21764000	-0.49301200
K	0.86498700	1.33983300	0.24053000	K	0.51549700	0.95397300	0.04460400
H	-2.63252500	0.91475000	2.63403800	H	-3.09958900	-0.17948400	2.34742700
H	-3.46275900	2.28716100	3.33546200	H	-3.83640200	0.92619800	3.48598500
H	-4.02108400	1.66211400	1.79940900	H	-4.44258500	0.88151600	1.84571300
H	1.69468700	-3.00331700	-3.92658600	H	6.00335400	3.27025800	-1.12040200
H	2.66149000	-1.59015300	-3.52798300	H	5.29497500	2.77911800	0.41466200
H	3.02935100	-3.15996700	-2.79626900	H	6.41565500	1.70515100	-0.43275800
H	-1.56126200	-1.33815900	-2.33935900	H	1.55076500	2.31072200	-2.18402700
H	-0.55433600	0.10939900	-2.21220400	H	2.08222600	3.21462300	-0.73478400
H	-0.40658400	-0.95090100	-3.60548700	H	2.66054700	3.65044700	-2.32359300
H	0.31038800	2.25801900	2.79199900	H	-0.08306300	0.84374200	2.79499600
H	0.75258100	3.71594300	1.85498000	H	0.43481100	2.53386200	2.52778800
H	-0.16008700	3.84633200	3.33713300	H	-0.46605900	2.09005400	3.96257500
H	6.36673600	3.43613200	0.48023300	H	2.01160300	-2.42936700	4.99408000
C	3.49207300	-1.04769600	-0.28056500	C	3.72736500	-0.89603400	0.14752600
C	4.02274400	-2.41541500	0.07905000	C	4.55201900	-1.79590000	-0.73624000
H	3.22287400	-3.13752100	-0.09507400	H	4.50113500	-1.40885900	-1.75471000
H	4.24230300	-2.42851000	1.15533900	H	4.12684400	-2.80421100	-0.74029000
O	2.35587400	-0.89366100	-0.75584800	O	3.46034400	0.27480300	-0.20842800
C	5.28878500	-2.80467500	-0.70946300	C	6.02247400	-1.85120400	-0.26256100
H	6.11677100	-2.11434600	-0.52087100	H	6.10560600	-2.26107300	0.74885500
H	5.60781900	-3.80882000	-0.41349400	H	6.59797500	-2.48820700	-0.94071800
H	5.08635600	-2.81697000	-1.78416300	H	6.47216900	-0.85367400	-0.26934000
H	-4.17934700	2.18416200	-2.87171300	H	-4.42532400	3.09230000	-2.46800000
H	-4.09348800	3.92153300	-3.25613300	H	-4.21562500	4.84021600	-2.19982500
H	-3.07218100	2.78064500	-4.13441900	H	-3.22610800	4.01914800	-3.40745200
H	-1.61726000	4.85467600	-3.20410600	H	-0.57065700	4.18464900	-1.37275300
H	1.40404500	-1.67289400	3.73892100	H	1.25735100	-2.85242600	-0.93782100
H	-1.07673700	-2.39674100	4.43981700	H	-1.10262700	-4.94411000	-2.58742400
H	-0.89970600	-3.92127400	3.57047300	H	-0.92877200	-3.88475600	-3.98471200
H	-2.20119900	-2.79183600	3.12075200	H	-2.34718200	-3.71603000	-2.93027700
O	-4.61686600	-1.88372600	-0.38458600	O	-5.15696100	-1.97440900	-0.47619300
C	-4.84243300	-3.07258800	-0.20294500	C	-5.22250900	-3.17036200	-0.22888700
C	-3.77129000	-4.01971600	0.29107500	C	-3.99096600	-3.96778300	0.15011900
H	-3.43799800	-4.64987600	-0.54458800	H	-3.89040200	-3.95077300	1.24458800
H	-2.90984500	-3.46698900	0.67468700	H	-4.07371900	-5.01688400	-0.15219900
H	-4.16418000	-4.69485900	1.06023300	H	-3.09438800	-3.51615400	-0.28701500
C	-6.21302200	-3.65545100	-0.47715800	C	-6.54484400	-3.90583500	-0.27136000
H	-6.84781100	-2.91587000	-0.96911400	H	-7.36664300	-3.20255800	-0.41934300
H	-6.13524500	-4.55750000	-1.09574100	H	-6.53374900	-4.63327800	-1.09364200
H	-6.67779700	-3.95875600	0.47012700	H	-6.69868200	-4.47575500	0.65321700
TS(Ic'$_m$-2'$_m$)				**2'$_m$**			
C	2.32251200	-3.38026700	0.06380100	C	-2.00734600	-3.84255300	0.69163500
C	0.12420600	-0.72142500	-2.36564300	C	0.35622500	-2.05771800	2.35918600
C	-0.59014400	-3.23593100	-0.74019500	C	1.71727300	3.12935300	3.27814900
C	-3.77959500	2.13962300	-3.38519300	C	-4.39962400	-0.10029000	0.37646800
C	4.80680800	-0.14215300	-0.34365100	C	-5.41855400	0.84558200	0.58603200
C	6.10980100	-0.06392400	-0.86057300	C	1.03907500	3.03137500	1.93830100
C	-2.67554500	2.54420900	-2.44602900	C	-0.15059800	3.91394300	1.66122300
C	-1.68959700	3.59042100	-2.89702700	C	-4.24448800	-0.62401400	-0.92196100
C	4.52262100	0.50376000	0.87260300	C	-6.26036400	1.23935200	-0.45460800
C	7.10174100	0.64187600	-0.18048500	C	-5.08533100	-0.22842500	-1.96419300
C	5.51552600	1.20178700	1.55597000	C	-0.64581700	-2.66622300	-3.10100600
C	1.41314300	-0.76577300	3.35597400	C	-6.09766100	0.70723900	-1.73573700
C	6.80826600	1.27596000	1.02872700	C	0.62860000	-2.74291200	-2.30089500
C	0.02440400	-1.21411100	2.98126900	C	1.81100000	-3.46715500	-2.88522400
C	-0.90845700	-1.66904100	4.07092600	C	3.38841300	1.50994800	-1.88130100
C	-3.10734700	1.99560700	2.26114700	C	2.12514800	4.60222300	-1.52344800
C	-2.90833000	4.94837100	0.65219600	C	0.36090400	2.20701500	-3.09785200
C	-0.14591900	3.49232400	1.91229300	H	-2.46821000	-4.20133600	1.62253900
H	2.11266100	-4.36432200	-0.36740800	H	-2.81433400	-3.78674700	-0.05329700
H	3.26558000	-3.44644800	0.62672300	H	-1.32343500	-4.63684900	0.35845200
H	1.56529000	-3.21549700	0.84422500	H	-5.53607100	1.28425500	1.57270600
H	6.33853700	-0.54073400	-1.80910600	H	-3.47604400	-1.37174900	-1.09935200
H	3.52221800	0.41860400	1.28585200	H	-0.20873400	4.73128000	2.38631700
H	-2.09554400	4.17770800	-3.72631300	H	-7.03973200	1.97350600	-0.26611800
H	8.10399200	0.70039900	-0.59641400	H	-0.09701300	4.32800700	0.65126100
H	-1.42803600	4.25661100	-2.07177200	H	-1.51109600	-2.87319600	-2.46542600
H	2.15198500	-1.17823300	2.66359900	H	-0.62897400	-3.37412500	-3.93481600
H	1.66088700	-1.06898100	4.37764400	H	-4.95790500	-0.66216600	-2.95340000
H	5.28544700	1.68377500	2.50278200	H	2.74126600	4.85333600	-0.64748700
H	-3.85671100	4.79644300	0.11604300	H	1.21634500	5.21965500	-1.45676100
H	-2.29271700	5.60884100	0.02266600	H	2.67801700	4.96651600	-2.40216400
H	-3.15536700	5.52798100	1.55418600	N	1.51873900	2.17919600	1.10467700

N	-2.63461600	1.95114300	-1.30677500	N	0.78406900	-2.21664000	-1.13847900
N	-0.43164100	-1.22654300	1.77926500	O	-0.33349600	-1.50574800	-0.66789500
O	0.46346900	-0.73448700	0.81947200	O	0.81868400	2.08481000	-0.11164400
O	-1.55606100	2.32143200	-0.48495400	Al	-1.05868800	-2.11815700	0.94032800
Al	0.79193100	-1.74731600	-0.72114900	Al	1.72886400	2.64909100	-1.66476100
Al	-1.99545200	3.23168600	1.11069900	K	2.19936100	-0.37942800	0.37816300
K	-2.51088900	-0.33004100	0.22327400	K	-1.40327200	0.94724500	-0.90066800
K	0.96965200	1.63963500	-0.28305600	H	0.63858700	-1.04058500	2.67627800
H	-1.56930900	-2.85074800	-1.07294800	H	0.00114200	-2.56003700	3.26992800
H	-0.32568200	-4.01979300	-1.46623400	H	1.27456500	-2.59277100	2.06965500
H	-0.74383800	-3.73361100	0.22685200	H	0.76865100	2.54837300	-4.06125200
H	-0.24999100	4.13641800	2.79827800	H	0.15431100	1.13273000	-3.24426300
H	0.33941600	2.57423800	2.28604900	H	-0.60607500	2.73135600	-3.00276600
H	0.57432300	4.02252000	1.26423100	H	4.04709800	1.53077200	-0.99849100
H	-4.02918300	1.63618700	1.77460100	H	3.20546000	0.45544900	-2.14792800
H	-2.56301700	1.12014500	2.65231300	H	3.98838700	1.91846600	-2.70835300
H	-3.44812400	2.54571300	3.15117900	H	-6.75202700	1.01689300	-2.54612200
H	-0.87863000	-0.28419900	-2.21909600	C	-3.47579000	-0.52275600	1.47306300
H	0.76005500	0.08256400	-2.77014900	C	-3.91201700	-0.66392500	2.74252800
H	-0.01337500	-1.43626800	-3.19168000	O	-2.19139500	-0.69681300	1.07788900
H	7.58248000	1.82426600	1.55869700	C	-3.06305400	-1.02935600	3.92354100
C	3.72213900	-0.85252100	-1.07705800	H	-3.24447800	-0.34584200	4.76478700
C	3.96828200	-2.03923100	-1.82489600	H	-3.28593300	-2.04148600	4.29162000
H	3.17605900	-2.70019100	-0.97356900	H	-1.99845200	-0.98996000	3.67856200
H	5.00332900	-2.38305900	-1.80399900	H	-4.97455500	-0.52172900	2.92292300
O	2.51553300	-0.50692600	-0.82236800	O	4.67189900	-1.22834000	0.96698500
C	3.26131000	-2.33770700	-3.14292100	C	5.88102700	-1.35041500	0.82898500
H	2.23568400	-1.96251400	-3.14787900	H	2.09662400	4.14573100	3.44613600
H	3.78647600	-1.87320900	-3.98801900	H	1.00915600	2.91381000	4.08958700
H	3.22649700	-3.41764500	-3.32693800	H	-1.08273400	3.33659900	1.73691500
H	-0.76420100	3.11400000	-3.25102800	H	2.55236800	2.42660600	3.34273800
H	1.48948300	0.32870700	3.30179500	H	-0.77771400	-1.65842600	-3.51751800
H	-0.47930300	-2.51875000	4.61797700	H	1.55677800	-4.51365100	-3.09795900
H	-1.07347000	-0.86663800	4.80243100	H	2.11417700	-3.01153600	-3.83744900
H	-1.87453300	-1.96939900	3.65629700	H	2.65929900	-3.44397000	-2.19588200
H	-4.41038800	1.36964900	-2.93275500	C	6.64487100	-0.56082200	-0.21195500
H	-4.40608900	3.00403100	-3.64099600	H	7.23781900	-1.23217000	-0.84508200
H	-3.36737800	1.75266400	-4.32695200	H	5.96017200	0.02507700	-0.82887300
O	-4.57291900	-2.02541300	0.07321000	H	7.35526000	0.11341600	0.28371300
C	-5.14923100	-3.10312400	0.01559100	C	6.67395300	-2.30178900	1.69979400
C	-4.38932600	-4.41098500	0.00050000	H	6.02501000	-2.75796700	2.44977700
H	-4.80302400	-5.09830500	-0.74641200	H	7.12470300	-3.08694900	1.07949300
H	-3.32720100	-4.24017300	-0.18965600	H	7.50010000	-1.77450100	2.19218000
H	-4.50296200	-4.89999400	0.97775100				
C	-6.66041400	-3.17698400	-0.03658200				
H	-7.04141500	-3.89753000	0.69678800				
H	-7.09559600	-2.19194100	0.14306800				
H	-6.97352700	-3.53600300	-1.02579000				
TS(Ic_m-Vc_m)				**Vc_m**			
C	4.02520800	-1.72820900	-3.03913200	C	-2.64435500	-4.57530600	0.78190700
C	3.83776600	1.18005500	-1.36337500	C	-3.42187100	-1.45442100	1.75709000
C	1.78224000	0.63270000	-3.90919300	C	-0.53212700	-2.81881700	2.72419000
C	0.02545100	4.46204700	-1.92206200	C	0.02926400	1.74646800	4.44512300
C	-4.22682700	-3.72261800	0.16893500	C	5.53062700	-1.93556600	0.07653000
C	-3.88601300	-2.47804400	-0.36475000	C	4.77243600	-1.16798300	-0.81423000
C	-4.95443400	-3.80178000	1.35728900	C	5.62148500	-1.57345300	1.41982300
C	0.35817400	3.81937800	-0.60246100	C	-0.44890200	1.99740600	3.04067500
C	1.33870800	4.51182700	0.30736400	C	-1.62058200	2.92123400	2.82749700
C	-5.34217900	-2.62425500	2.00164400	C	4.94986500	-0.43065500	1.86491400
C	-4.26212400	-1.29038900	0.27400500	C	4.08395900	-0.02582000	-0.38299300
C	1.66825800	-3.36113400	0.11461400	C	-1.67793900	-3.06114300	-2.68784200
C	0.73746700	-2.99682400	-1.01354700	C	-0.34320400	-3.11449000	-1.98849700
C	-5.00098400	-1.38331600	1.46300800	C	4.19215400	0.33083600	0.97366800
C	-0.27797300	-4.01114200	-1.46560000	C	0.80754100	-3.80181800	-2.67268400
C	-2.76885000	0.82222800	1.00017100	C	2.84414500	0.11707700	-2.61477100
C	-1.84994400	3.48018000	2.93668100	C	1.37225300	4.17148300	0.23743300
C	-0.25484000	0.46059600	3.35435600	C	-0.46329500	2.45100500	-2.06184400
H	4.77439600	-1.38172200	-3.76641100	H	-3.04147000	-5.11028600	1.65756500
H	4.58905000	-2.19997000	-2.21869400	H	-3.46573500	-4.53537800	0.04995800
H	3.46466100	-2.53443100	-3.53409100	H	-1.86983900	-5.22699600	0.35142500
H	-3.93202800	-4.63253500	-0.34977900	H	6.05011400	-2.81935700	-0.28571800
H	-3.33187800	-2.39523700	-1.29377700	H	4.72205700	-1.47326100	-1.85445300
H	-5.22253900	-4.76880900	1.77561400	H	6.21094900	-2.16941700	2.11157300
H	1.40889200	5.57616100	0.06419600	H	-1.80346800	3.53217700	3.71661300
H	1.05057100	4.39300200	1.35429800	H	-1.44681000	3.57109600	1.96617800
H	2.64063400	-2.88092900	-0.01718600	H	-2.47919700	-3.36947900	-2.01074700

H	1.80126500	-4.44609800	0.17337400	H	-1.68340800	-3.70510400	-3.57224700
H	-5.91335200	-2.67217400	2.92592400	H	5.01896300	-0.12891500	2.90755200
H	-5.31182000	-0.48051700	1.98277400	H	3.66253600	1.21098800	1.32669500
H	-2.27951100	4.15030800	2.17984100	H	1.89181600	4.06857300	1.20122200
H	-1.07964100	4.05570600	3.47058400	H	0.52586200	4.85349100	0.40991000
H	-2.64553500	3.27200500	3.66510600	H	2.06123400	4.69965400	-0.43541000
N	-0.21689200	2.69852600	-0.34160300	N	0.17400500	1.39104100	2.09432700
N	0.73247200	-1.86234000	-1.61719300	N	-0.11457700	-2.60417200	-0.83165500
O	1.64950800	-0.91695800	-1.12547300	O	-1.21459200	-1.94523500	-0.25303900
O	0.17482100	2.11672400	0.88103500	O	-0.35368300	1.61776700	0.81109700
Al	2.84167800	-0.23912300	-2.42453600	Al	-1.94943500	-2.76874100	1.28212400
Al	-1.09757000	1.82371700	2.16006400	Al	0.75820200	2.41058600	-0.45487900
K	-0.77110400	0.40011200	-2.09949500	K	1.19147400	-0.91621700	0.92797600
K	2.16904400	0.36705600	1.08117200	K	-2.32473000	0.42900700	-0.47560300
H	1.28188800	1.57671900	-3.63331400	H	-0.27322900	-1.83603100	3.15202000
H	2.47309500	0.90477000	-4.72122700	H	-0.91086600	-3.41001100	3.57147400
H	1.03399800	-0.02743300	-4.37678000	H	0.40310400	-3.31830000	2.42134500
H	-0.91295300	0.23152400	4.20365200	H	-0.02566100	3.06770000	-2.85996400
H	-0.05550000	-0.50705300	2.86719600	H	-0.64223800	1.46735500	-2.52861000
H	0.68979700	0.81306700	3.79982900	H	-1.44431400	2.90937800	-1.85216600
H	-2.54216300	1.71379600	0.42035700	H	2.13230500	0.72671300	-3.17712000
H	-2.06158900	-0.00070400	1.00456100	H	2.35625600	-0.83630300	-2.38428600
H	-3.38755400	0.93893200	1.88686400	H	3.70749300	-0.08004500	-3.26160300
H	3.21010800	2.00590000	-0.98715000	H	-3.08145400	-0.46583800	2.10905800
H	4.45795900	0.81772500	-0.52641300	H	-4.16400800	-1.29639200	0.95652400
H	4.54771600	1.65812900	-2.05530600	H	-3.99033500	-1.87728100	2.59917000
C	-3.87179600	0.04170500	-0.39127900	C	3.22517000	0.85886700	-1.31749400
C	-5.07006300	1.02295100	-0.48293300	C	4.06879900	2.12922000	-1.64135800
H	-5.83620100	0.49472100	-1.06993600	H	4.18103200	2.68927800	-0.70523100
O	-3.13545300	-0.04633600	-1.44190200	O	2.04076100	1.16656900	-0.61680400
C	-4.74442100	2.34439000	-1.17715800	C	3.51793200	3.05508500	-2.73176100
H	-5.65178300	2.94208300	-1.32266600	H	4.13333500	3.95949300	-2.80105300
H	-4.04214400	2.95249900	-0.59325600	H	3.52681000	2.57613000	-3.71694200
H	-4.29283100	2.15273400	-2.15486200	H	2.49239500	3.37580600	-2.52450600
H	-5.50970600	1.20651300	0.50407700	H	5.07745600	1.80539100	-1.93164300
O	4.32822700	-0.56909100	2.33543500	O	-4.78610100	1.19677300	-1.14692600
C	5.43054400	-1.09865900	2.39716800	C	-5.99748300	1.36572800	-1.10447400
C	6.07653200	-1.73208700	1.18545100	C	-6.86432900	0.63267800	-0.10442500
C	6.20063400	-1.14551600	3.69871600	C	-6.68727200	2.31866600	-2.05612100
H	7.09912100	-0.52033800	3.61507400	H	-7.11649400	3.15688600	-1.49226400
H	6.54374300	-2.16494700	3.91121300	H	-7.52085100	1.82079400	-2.56590500
H	-0.70479100	3.86753200	-2.47777000	H	0.87344000	1.05195600	4.45055900
H	-0.38859500	5.46624200	-1.76630600	H	0.33978500	2.68546800	4.92178900
H	2.34102000	4.07830700	0.18695000	H	-2.53364700	2.34370300	2.62620500
H	-0.86874700	-3.61862700	-2.29702600	H	1.70649300	-3.76416100	-2.05179500
H	0.92877000	4.57746300	-2.53532400	H	-0.77683700	1.32554200	5.06085300
H	-0.95955000	-4.27192600	-0.64493400	H	1.02421700	-3.33175100	-3.64148700
H	0.21539100	-4.93794100	-1.78600500	H	0.56257800	-4.85274000	-2.87495500
H	1.25262000	-3.03494200	1.07952800	H	-1.90254400	-2.03701100	-3.01592000
H	7.11291400	-1.39235500	1.07430600	H	-7.51363400	1.33394200	0.43309900
H	6.11532900	-2.82100900	1.32175300	H	-7.52507200	-0.06550700	-0.63479000
H	5.51257300	-1.50463100	0.27851000	H	-6.24741600	0.07537400	0.60354300
H	5.58157100	-0.77995600	4.52026100	H	-5.97651600	2.70290400	-2.79023600
TS(Ic'$_m$-Vc'$_m$)				**Vc'$_m$**			
C	-0.81532800	-4.34875800	1.59374800	C	1.24265000	-4.28801600	0.03916400
C	-2.66798900	-1.56384000	0.72730900	C	2.94679800	-0.45558300	-2.56092100
C	0.06274900	-1.26883900	2.79594400	C	-0.31305000	-2.29866700	-2.19725400
C	0.31989900	4.05617500	1.73787800	C	-1.01069400	3.22843100	-3.33934000
C	0.20993200	3.35181000	0.41176500	C	-0.55115800	3.07236500	-1.91473500
C	-0.86767900	3.79438500	-0.54137600	C	0.60720400	3.90521700	-1.42786400
C	6.15665700	-0.28803500	3.93682000	C	-6.72228000	-1.61546100	-2.48626300
C	0.74374000	-3.54203800	-2.47725300	C	-0.33312600	-2.60097000	3.39965500
C	1.73765500	-3.11697400	-1.42959300	C	-1.47541900	-2.62457100	2.41749300
C	3.17078200	-3.54690200	-1.59295400	C	-2.79546600	-3.20153900	2.85156200
C	3.95951900	1.16675100	-1.58487200	C	-3.49370300	1.66926300	1.54403900
C	2.37865300	3.85336900	-2.81682700	C	-2.05087800	4.68951300	1.31003600
C	1.52217500	0.74669300	-3.81290700	C	-0.61945700	2.25015100	3.13572700
H	-1.39943000	-4.58058000	2.49481500	H	1.77785300	-4.83608300	-0.74925000
H	-1.30602500	-4.86135300	0.75520200	H	1.88660700	-4.31584300	0.93059300
H	0.16678500	-4.82495300	1.72614000	H	0.34928200	-4.88442100	0.27612500
H	-1.08349800	4.85981400	-0.40992200	H	0.86707900	4.67817400	-2.15721500
H	-0.57687000	3.60883400	-1.57656900	H	0.36531200	4.37671700	-0.47147000
H	-0.27035300	-3.55489500	-2.07493100	H	0.59934100	-2.89424000	2.91031800
H	0.99729900	-4.53338600	-2.86705400	H	-0.52816500	-3.26821200	4.24455500
H	2.64982100	4.49469600	-1.96538700	H	-2.50225500	4.95320300	0.34211900
H	1.44650600	4.26263300	-3.23440700	H	-1.12143900	5.27295000	1.39433800

H	3.15327000	4.01361900	-3.58151900	H	-2.72919800	5.08374000	2.08152200
N	1.04239800	2.39638900	0.19592800	N	-1.18390500	2.22217700	-1.18782400
N	1.46412000	-2.39679300	-0.39954700	N	-1.40513300	-2.17005600	1.21741200
O	0.11978200	-1.96633400	-0.31631500	O	-0.16750800	-1.59250500	0.88530000
O	0.87588300	1.71277600	-1.02435900	O	-0.68676900	2.08350400	0.11961900
Al	-0.64027000	-2.39947600	1.30943500	Al	0.75959800	-2.43618700	-0.50202200
Al	2.22848800	1.92542700	-2.32128700	Al	-1.76533300	2.72330300	1.52883700
K	2.24136600	0.02119400	0.76188600	K	-2.21427800	-0.26412100	-0.62224500
K	-0.91038700	0.02808600	-2.01094500	K	1.23147100	0.66484100	1.22683300
H	0.00071000	-0.18510500	2.61309300	H	-0.41647800	-1.27766700	-2.59984800
H	-0.52746300	-1.44937400	3.70538100	H	0.16595200	-2.87939700	-2.99949200
H	1.10233100	-1.51071400	3.06752000	H	-1.32330100	-2.72695600	-2.09522800
H	2.23506700	0.79119800	-4.64989600	H	-1.09307900	2.68522600	4.02861900
H	1.44119600	-0.32611100	-3.56618300	H	-0.53625500	1.17218700	3.35729000
H	0.56012000	1.07035600	-4.24574100	H	0.39872600	2.67660900	3.12139600
H	4.27718800	1.62733100	-0.63540800	H	-4.04895300	1.72529900	0.59396200
H	3.98626900	0.07094200	-1.46035700	H	-3.38625200	0.60647200	1.81699500
H	4.76060800	1.39557500	-2.30384400	H	-4.16219300	2.10168700	2.30379500
H	-2.11457900	-0.64876200	0.90725600	H	2.33375700	0.44914900	-2.48595700
H	-2.38888800	-2.21870600	-0.09132900	H	2.35764300	-1.21186700	-3.08822600
H	-3.15314800	-2.01845200	1.58761900	H	3.82907700	-0.22818200	-3.16915500
C	5.62120500	-0.09234300	2.53485500	C	-5.89003900	-0.94643600	-1.41285700
C	6.62739800	0.18565800	1.43950100	C	-6.62309600	-0.39840800	-0.20736700
H	6.12101700	0.45230900	0.50917900	H	-5.94665700	0.18299000	0.42301100
O	4.42166500	-0.15957100	2.30227500	O	-4.67495500	-0.85805000	-1.52023600
H	7.31318700	0.98808000	1.73615900	H	-7.47232900	0.22195900	-0.51759600
O	-3.32395500	-0.15265800	-1.38589600	O	2.10814400	-1.23249600	-0.44137300
C	-3.98459200	-0.62455600	-0.38955800	C	3.30154000	-0.98941100	-1.16044100
C	-4.53150500	0.40498600	0.61084400	C	4.09521900	0.04055100	-0.32376500
C	-5.01685900	-1.73341400	-0.71491300	C	4.11610700	-2.30809700	-1.28580500
C	-5.16161500	0.06346800	1.81652500	C	4.55488600	1.26591700	-0.82332600
C	-4.43044300	1.76148200	0.27868100	C	4.33136400	-0.23803000	1.03635200
H	-5.88663700	-1.20642200	-1.13516600	H	3.49322500	-3.02324700	-1.83887200
H	-5.36714900	-2.22664600	0.19870700	H	4.23152900	-2.72428900	-0.27815200
C	-4.53178300	-2.76595100	-1.73112200	C	5.49038700	-2.20215400	-1.95663100
C	-5.65838700	1.04791200	2.67068700	C	5.21073100	2.18725700	0.00276000
H	-5.25906700	-0.98097000	2.10105200	H	4.40560000	1.51760800	-1.86811400
C	-4.92819500	2.75107000	1.12908300	C	4.98670000	0.67472000	1.86336300
H	-3.96714800	2.01514200	-0.66941300	H	3.98667400	-1.18380100	1.44595100
H	-3.71898600	-3.38512700	-1.33024000	H	6.13844600	-1.48600000	-1.43888600
H	-5.34470500	-3.44330100	-2.01683100	H	5.99472400	-3.17500000	-1.94458900
H	-4.16460700	-2.26445600	-2.63142300	H	5.41446800	-1.88849500	-3.00373200
C	-5.54147400	2.39855200	2.33190700	C	5.42579600	1.90002600	1.34915300
H	-6.13832300	0.76021500	3.60314800	H	5.55340300	3.13091300	-0.41437200
H	-4.84452600	3.79849800	0.84735500	H	5.16186500	0.42809100	2.90814600
H	-5.93004400	3.16554900	2.99711400	H	5.93541400	2.61418400	1.99031500
H	1.11754900	3.61970300	2.34525200	H	-1.85129400	2.56232800	-3.55163300
H	0.52999000	5.12361800	1.59207100	H	-1.32221300	4.26323200	-3.53297500
H	-1.79874700	3.24666100	-0.33864900	H	1.49516800	3.27920200	-1.26706500
H	3.78854100	-3.16482400	-0.77598400	H	-3.52548500	-3.14982200	2.03939000
H	-0.62595300	3.98839500	2.29167700	H	-0.19511700	3.00428200	-4.04009800
H	3.57755700	-3.18205300	-2.54517100	H	-3.19091000	-2.65820200	3.72030500
H	3.24467100	-4.64173900	-1.60993900	H	-2.67811500	-4.24983100	3.15549100
H	0.77102700	-2.84800500	-3.32971400	H	-0.19282800	-1.58698300	3.79896500
H	5.35559000	-0.60206300	4.60869100	H	-6.07505600	-2.06969500	-3.23898100
H	7.24236600	-0.70901200	1.27429000	H	-7.03750900	-1.23096200	0.37661300
H	6.96513900	-1.02876100	3.94390800	H	-7.38011200	-2.37601800	-2.04889600
H	6.58717500	0.65407100	4.30028900	H	-7.37218900	-0.87204600	-2.96577700