

Supporting Information for:

Double insertion of CO₂ into an Al–Te multiple bond

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General Experimental Procedures.

All manipulations were performed under dry nitrogen using standard Schlenk-line techniques, or in a conventional nitrogen-filled glovebox. Solvents were dried over appropriate drying agents and degassed prior to use. NMR spectra were recorded using a Jeol JNM-ECZ500S 500 MHz spectrometer equipped with a ROYAL digital auto tune probe S, operating at 500.1 (^1H), 125.7 ($^{13}\text{C}\{^1\text{H}\}$), 95.4 (^{77}Se) and 157.8 (^{125}Te) MHz. Spectra were recorded at 298 K (unless stated otherwise) and proton and carbon chemical shifts were referenced internally to residual solvent resonances. Coupling constants are quoted in Hz. $\text{K}[\text{Al}(\text{NON}^{\text{Dipp}})]$ (**A**),^{S1} was prepared according to the literature procedure. All other chemicals were purchased from Sigma-Aldrich and used without further purification.

Synthesis of $\text{K}[\text{Al}(\text{NON}^{\text{Dipp}})(\text{Te})(\text{THF})]$, ($\text{K}[1\text{-Te}\cdot\text{THF}]$)

A catalytic amount of tri-*n*-butylphosphine (<0.1 mL) was added to a stirred slurry of tellurium (40 mg, 0.31 mmol) in toluene. A toluene solution of $\text{K}[\text{Al}(\text{NON}^{\text{Dipp}})]$ (**A**) (172 mg, 0.31 mmol) was added drop wise to the tellurium/phosphine mixture at room temperature and the solution stirred for 18 hours. The resulting suspension was allowed to settle, and the brown/green solution was decanted away to afford a white solid. The solid was washed using hexane and recrystallized from THF at room temperature to yield colourless crystals $\text{K}[1\text{-Te}\cdot\text{THF}]$. Yield 76 mg, 32.4 %. It was not possible to obtain accurate elemental analysis for this compound due to its extreme sensitivity to oxygen, moisture and possibly light. Samples prepared for analysis and flame-sealed under vacuum in a glass ampoule visibly changed colour from white to grey over a 4-day period, indicating decomposition. ^1H NMR ($\text{THF-}d_8$): δ 6.97 (d, $J = 7.9$, 3H, C_6H_3), 6.90 (t, $J = 6.8$, 2H, C_6H_3), 3.78 (sept, $J = 6.7$, 4H, CHMe_2), 1.38 (d, $J = 6.8$, 12H, CHMe_2), 1.19 (d, $J = 6.8$, 12H, CHMe_2), 0.02 (s, 12H, SiMe_2). $^{13}\text{C}\{^1\text{H}\}$ ($\text{THF-}d_8$): δ 147.7, 145.5, 123.7, 123.2 (C_6H_3), 28.7 (CHMe_2), 26.9, 24.8 (CHMe_2), 2.8 (SiMe_2).

Figure S1 ^1H NMR spectrum (500 MHz, THF-d_8 , 298 K) of $\text{K}[\text{Al}(\text{NON}^{\text{Dipp}})(\text{Te})(\text{THF})]$ ($\text{K}[\mathbf{1}\text{-Te}\cdot\text{THF}]$)

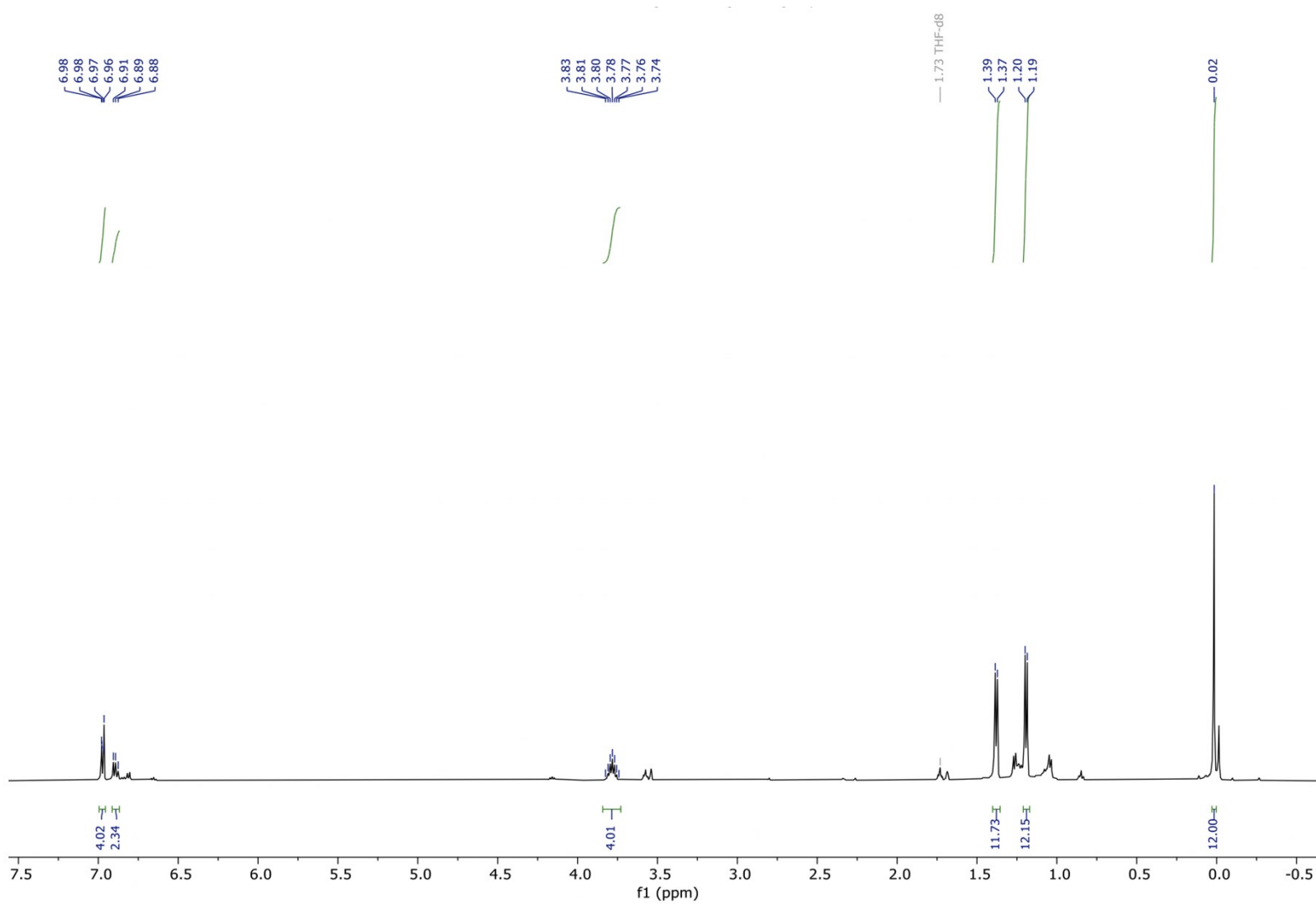


Figure S2 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, $\text{THF-}d_8$, 298 K) of $\text{K}[\text{Al}(\text{NON}^{\text{Dipp}})(\text{Te})(\text{THF})]$ ($\text{K}[\mathbf{1}\text{-Te}\cdot\text{THF}]$)

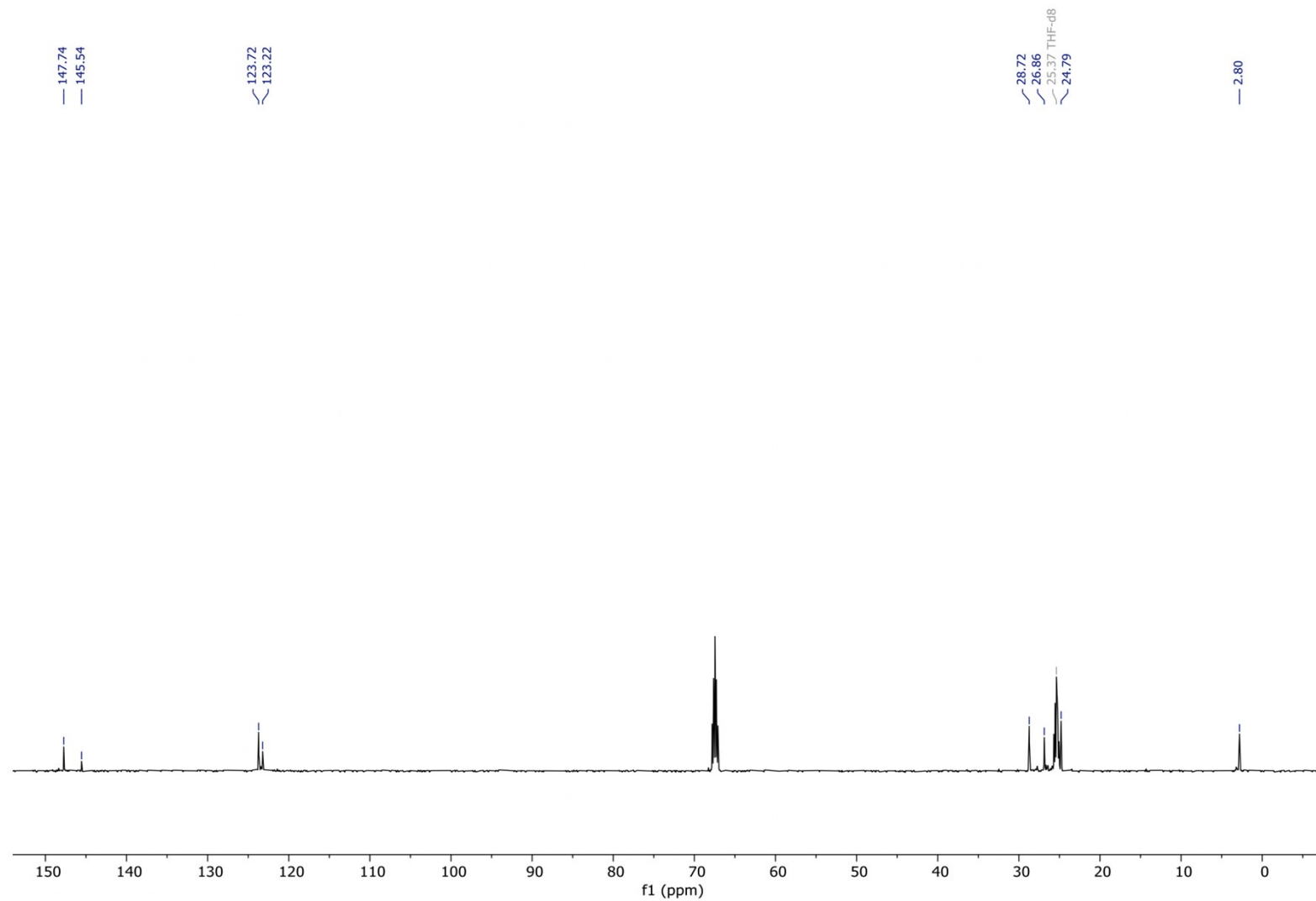


Figure S3 ORTEP (displacement ellipsoids 30 %) of $K[Al(NON^{Dipp})(Te)(THF)]$ ($K[1-Te \cdot THF]$)

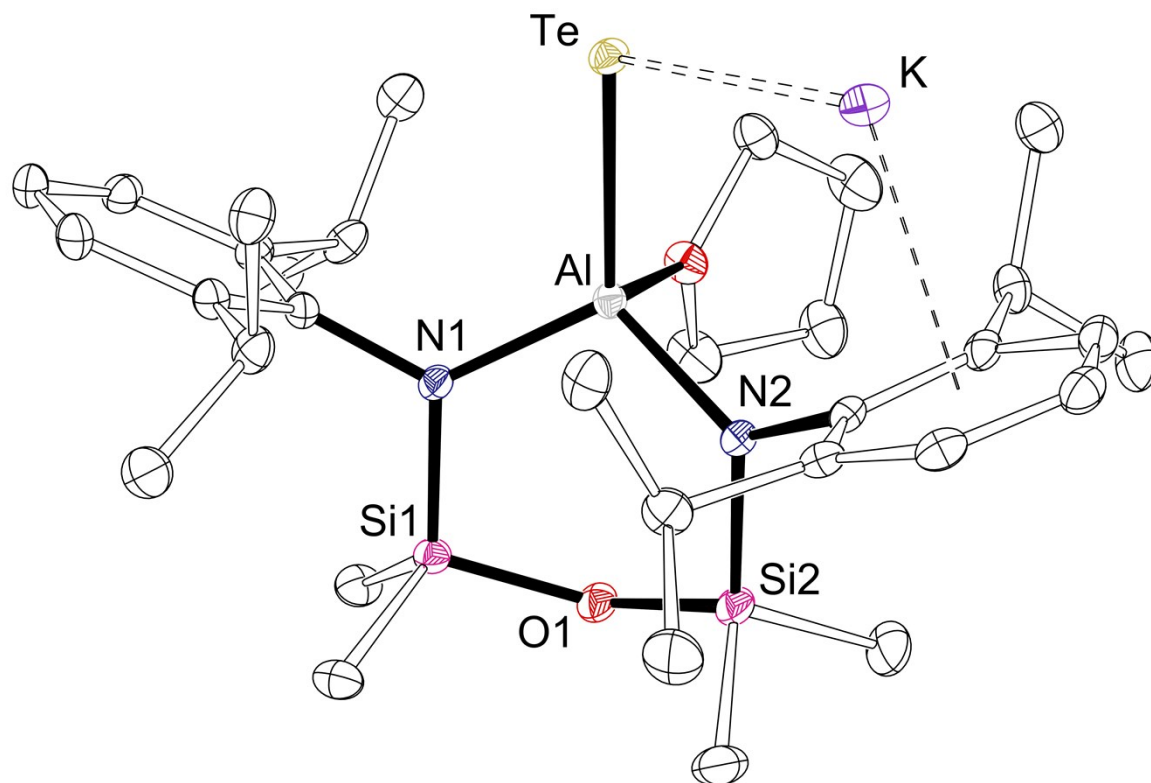
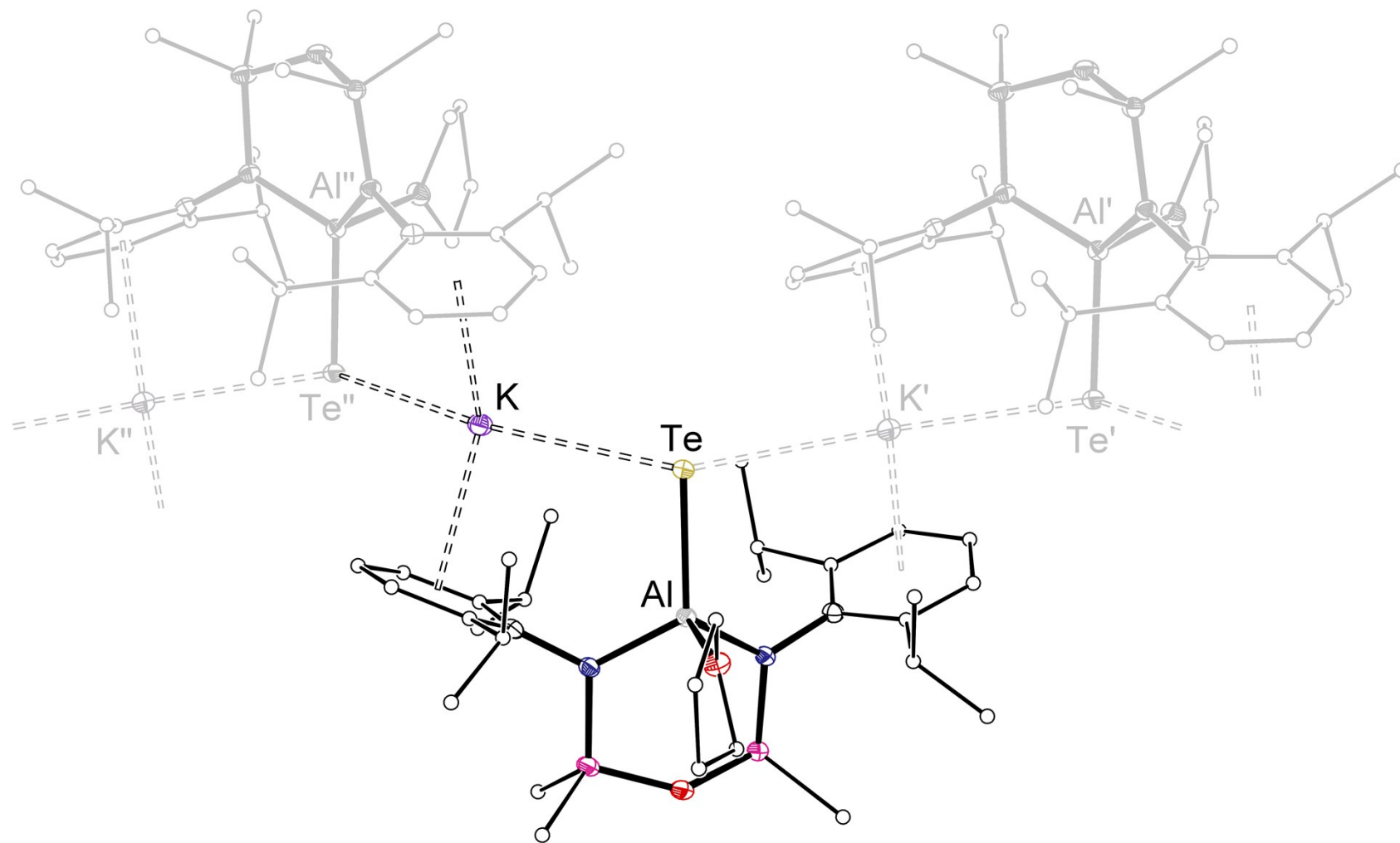


Figure S4 Section of the polymeric chain of (K[1-Te·THF]). ' = $1.5-x, 0.5+y, 0.5-z$; '' = $1.5-x, -0.5+y, 0.5-z$.



Synthesis of $[K(Et_2O)_3][Al(NON^{DiPP})(Te\{C(O)O\}_2)]$ (2).

A solution of $K[1-Te\cdot THF]$ (80 mg, 0.11 mmol) was prepared in a 50:1 mixture of THF: C_6D_6 and added to a J. Youngs NMR tube. The THF/ C_6D_6 solution was degassed and one atmosphere of CO_2 was added to the reaction vessel at room temperature. Reaction progress was monitored by 1H and $^{13}C\{^1H\}$ NMR spectroscopy and shown to be complete within 2 days at room temperature. The volatiles were removed *in vacuo* and the brown residue dissolved in Et_2O . Filtration through celite gave a yellow solution, from which colourless crystals were grown at $-30\text{ }^\circ C$. Yield 15 mg, 18.3 %. Samples of the crystals stored in the dark in a nitrogen filled glovebox at $-30\text{ }^\circ C$ decomposed over 3 days, indicating extreme instability that precluded the preparation of samples for elemental analysis. 1H NMR (500 MHz, THF- d_8): δ 6.89 (d, $J = 7.5$, 4H, C_6H_3), 6.78 (t, $J = 7.5$, 2H, C_6H_3), 3.91 (sept, $J = 6.8$, 4H, $CHMe_2$), 1.26 (d, $J = 6.8$, 12H, $CHMe_2$), 1.12 (d, $J = 6.8$, 12H, $CHMe_2$), 0.08 (s, 12H, $SiMe_2$). $^{13}C\{^1H\}$ NMR (126 MHz, THF- d_8): δ 164.5, 157.2 (C_6H_3), 155.0 ($J_{Te-C} = 327$, $Te\{^{13}C(O)O\}_2$), 147.5, 123.7 (C_6H_3), 28.0 ($CHMe_2$), 26.3, 26.2 ($CHMe_2$), 2.7 ($SiMe_2$). ^{125}Te NMR (158 MHz, THF): $\delta -17.8$ (d, $J_{Te-C} = 327$, $Te\{C(O)O\}_2$).

Figure S5 ^1H NMR spectrum (500 MHz, $\text{THF-}d_8$, 298 K) of $[\text{K}(\text{Et}_2\text{O})_3][\text{Al}(\text{NON}^{\text{Dipp}})(\text{Te}\{^{13}\text{C}(\text{O})\text{O}\}_2)]$ (**2**)

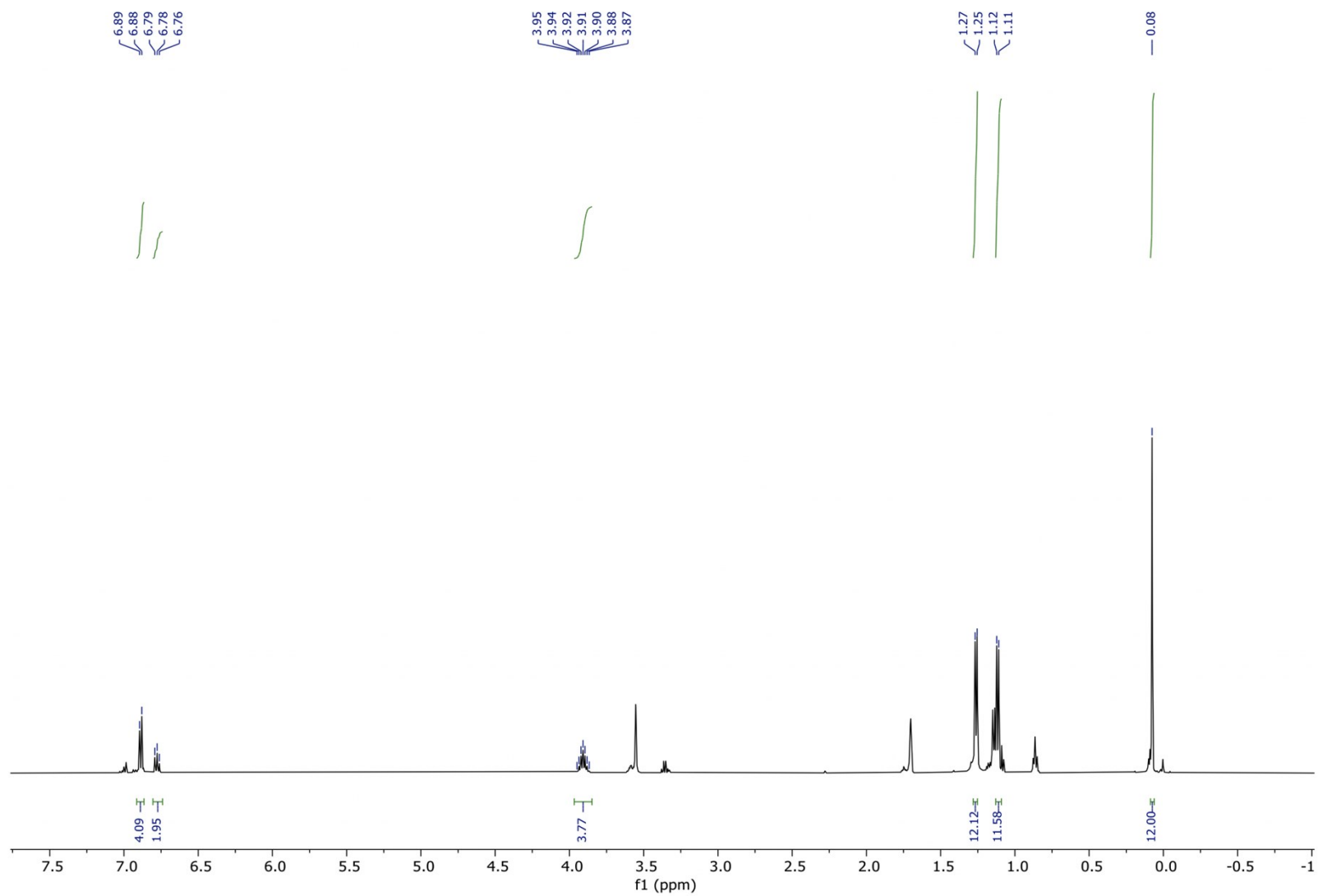


Figure S6 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, $\text{THF-}d_8$, 298 K) of $[\text{K}(\text{Et}_2\text{O})_3][\text{Al}(\text{NON}^{\text{Dipp}})(\text{Te}\{^{13}\text{C}(\text{O})\text{O}\}_2)]$ (**2**)

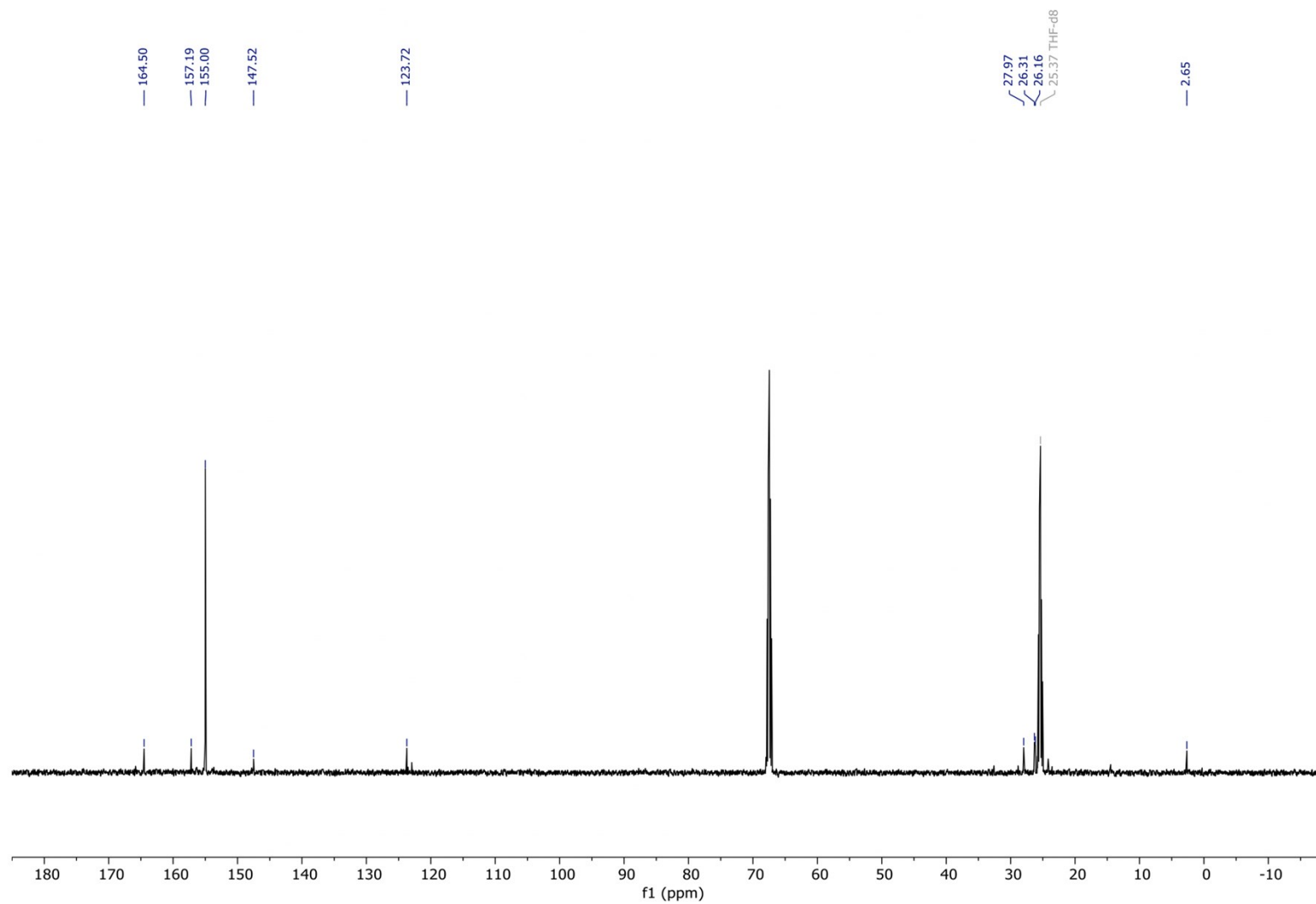


Figure S7 Expansion of $^{13}\text{C}\{^1\text{H}\}$ $[\text{Te}^{13}\text{C}(\text{O})\text{O}]_2$ resonance from $[\text{K}(\text{Et}_2\text{O})_3][\text{Al}(\text{NON}^{\text{Dipp}})(\text{Te}\{^{13}\text{C}(\text{O})\text{O}\}_2)]$ (**2**) showing $^1J_{\text{TeC}}$ coupling

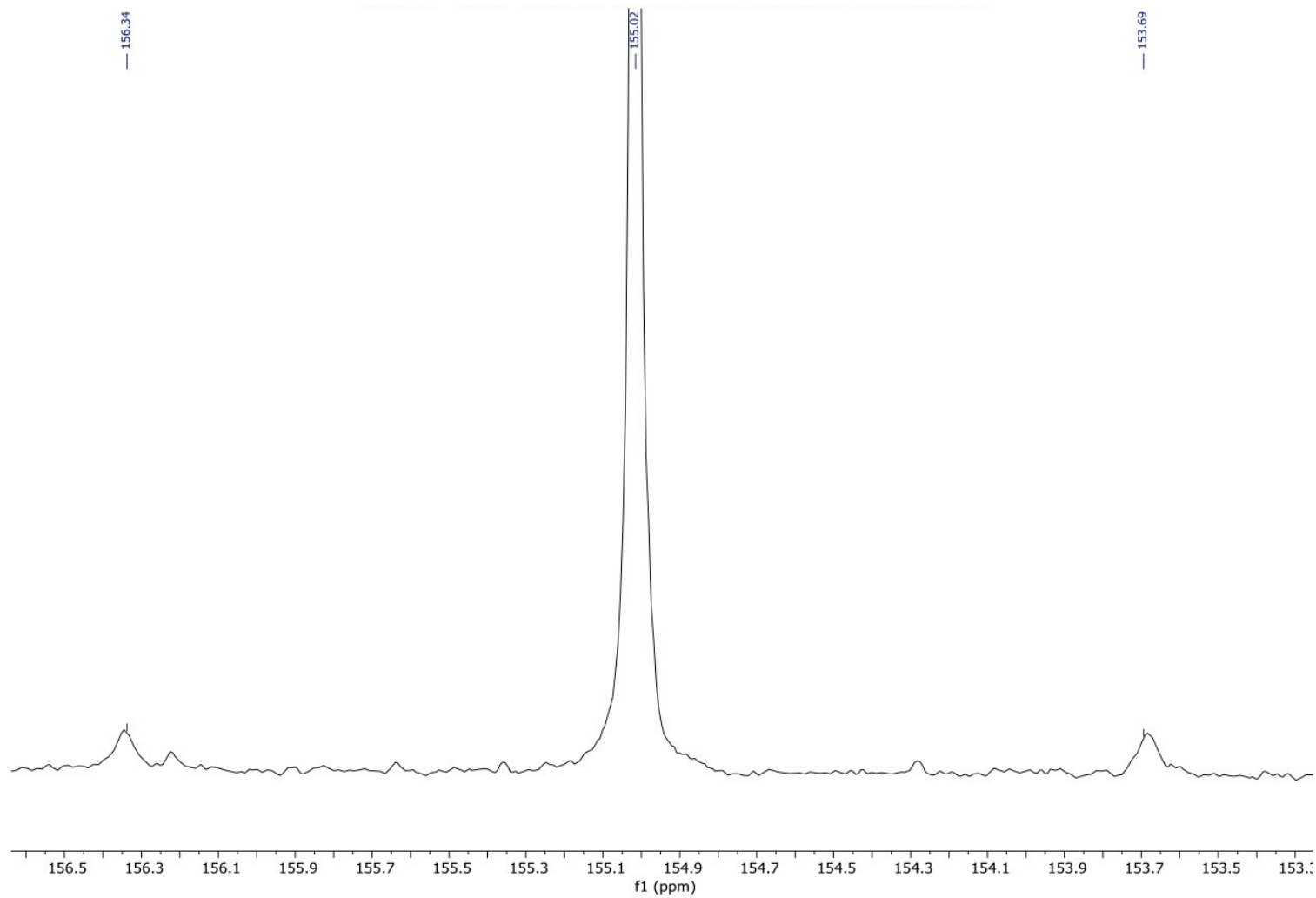


Figure S8 ^{125}Te NMR spectrum (158 MHz, THF- d_8 , 298 K) of $[\text{K}(\text{Et}_2\text{O})_3][\text{Al}(\text{NON}^{\text{Dipp}})(\text{Te}^{13}\text{C}(\text{O})\text{O})_2]$ (**2**)

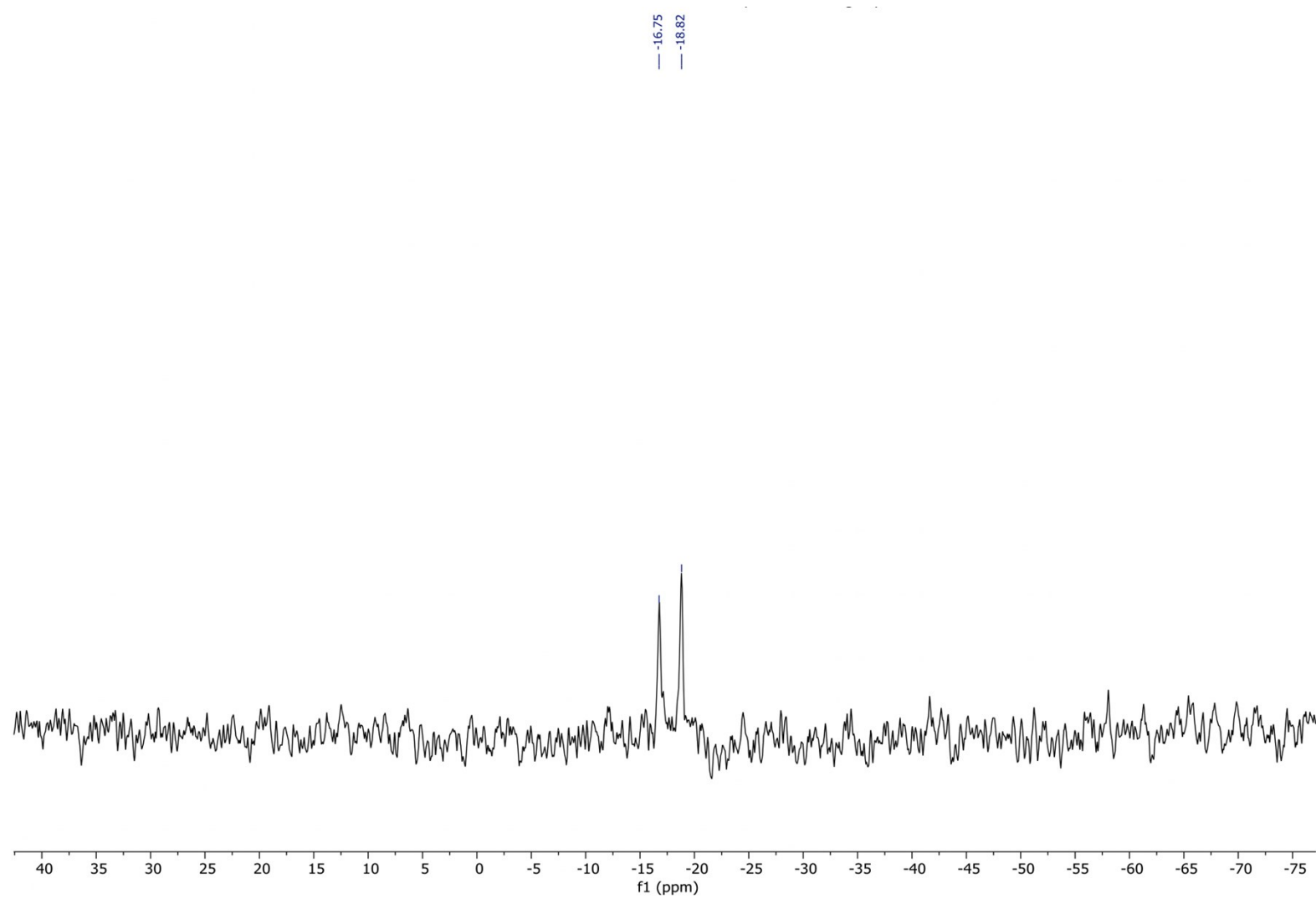


Figure S9 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, $\text{THF-}d_8$, 298 K) of reaction of $\text{K}[\text{Al}(\text{NON}^{\text{Dipp}})(\text{Te})(\text{THF})]$ ($\text{K}[1\text{-Te}\cdot\text{THF}]$) with $^{13}\text{CO}_2$ showing formation of intermediate at δ_c 142.1. Peak at δ_c 155.0 corresponds to $[\text{Te}\{^{13}\text{C}(\text{O})\text{O}\}_2]$ resonance from $[\text{K}(\text{Et}_2\text{O})_3][\text{Al}(\text{NON}^{\text{Dipp}})(\text{Te}\{^{13}\text{C}(\text{O})\text{O}\}_2)]$ (**2**)

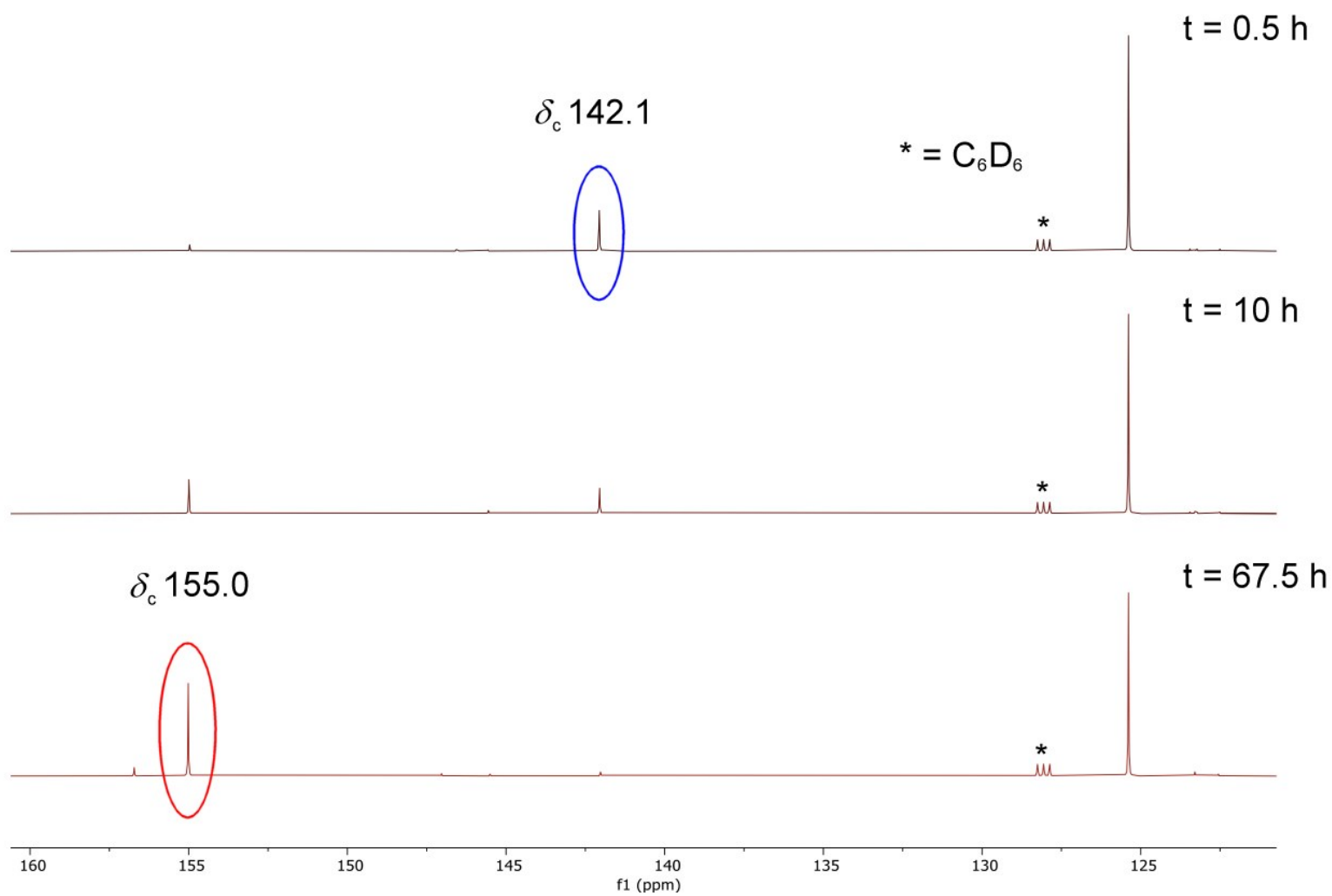


Figure S10 Expansion of $^{13}\text{C}\{^1\text{H}\}$ resonance at $\delta_{\text{C}} 142.1$ showing $^1J_{\text{TeC}}$ coupling

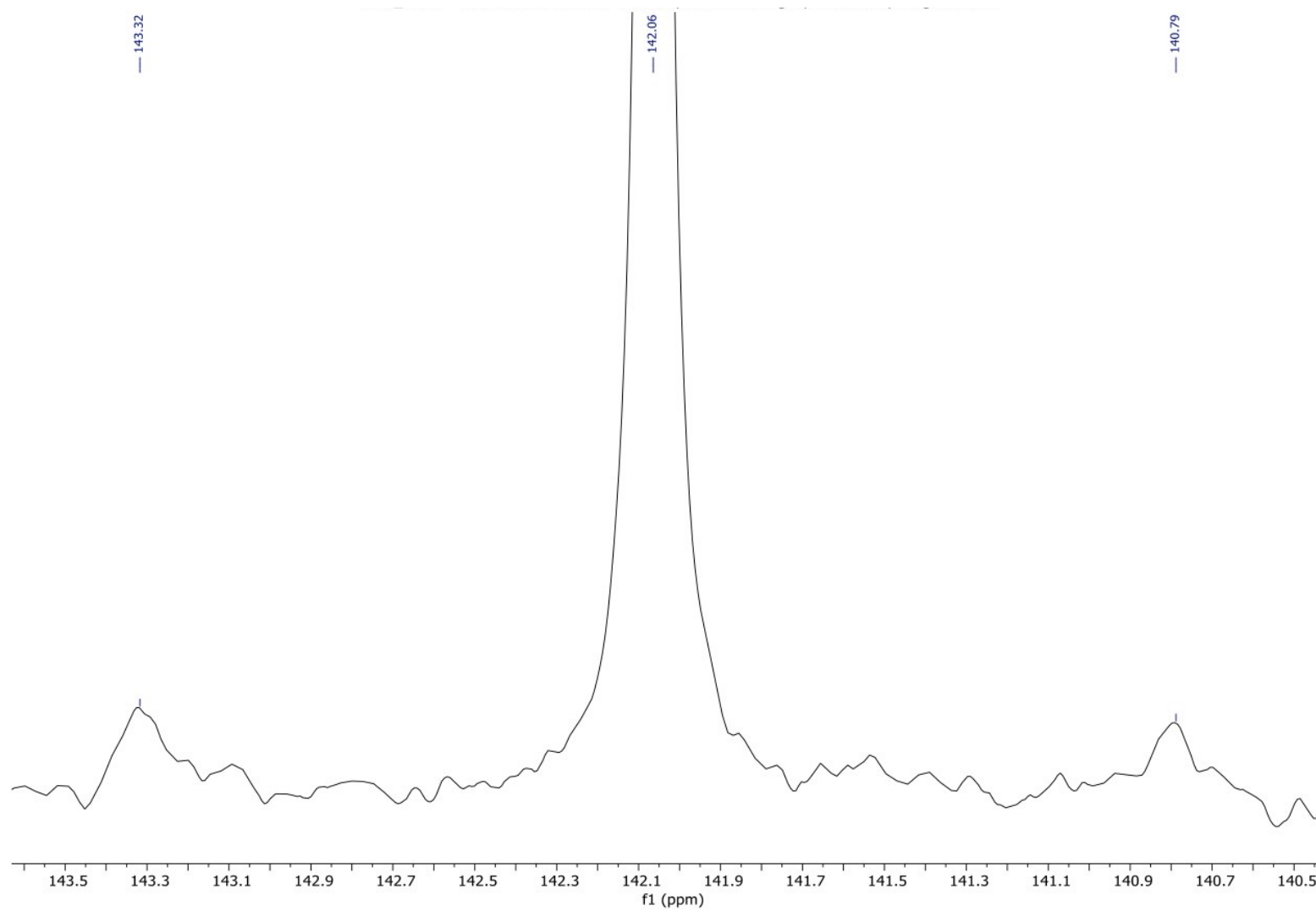
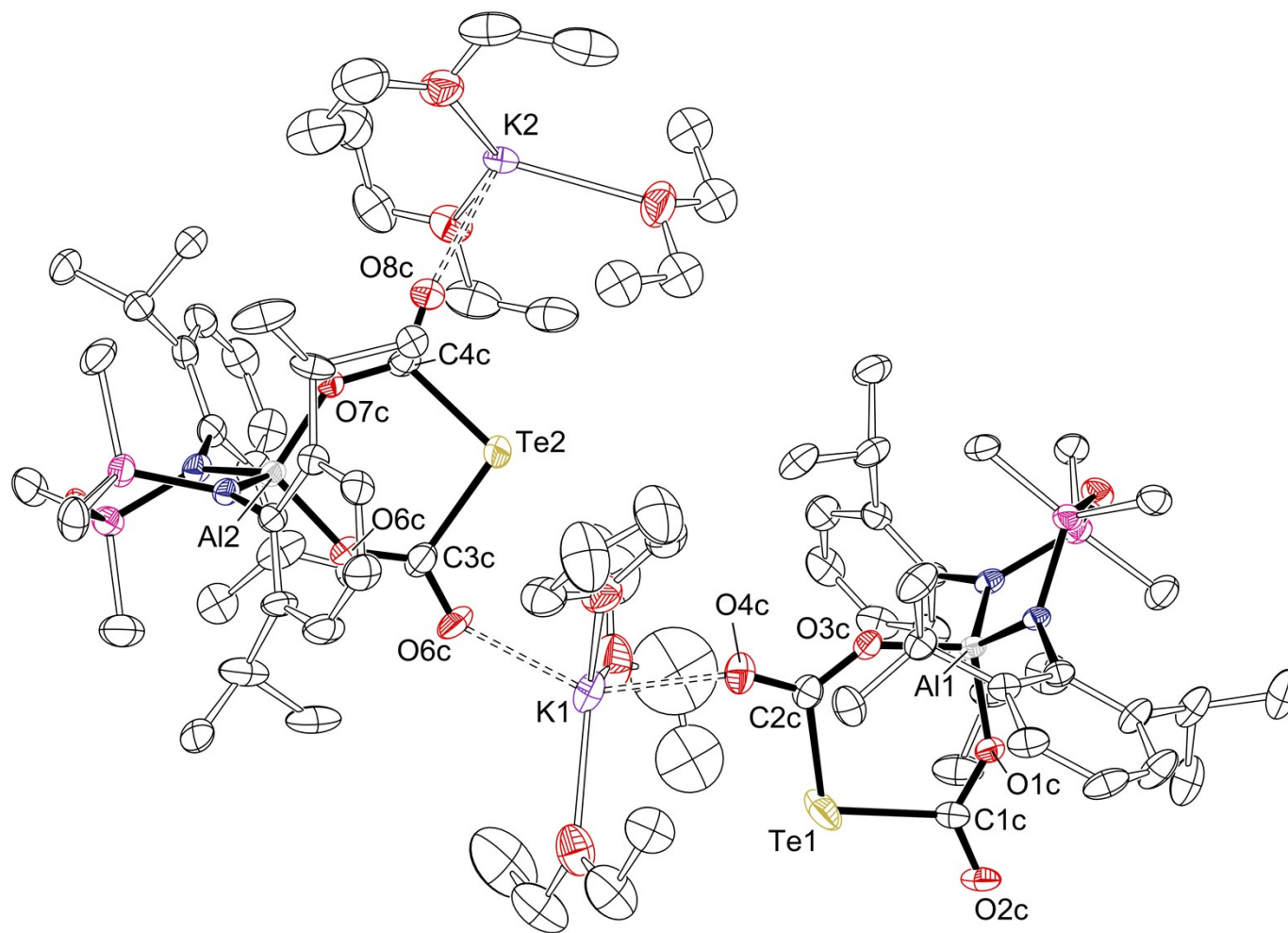


Figure S11 ORTEP (displacement ellipsoids 30 %) of $[K(Et_2O)_3][Al(NON^{Dipp})\{(OC(O)_2Te)\}][K(Et_2O)_2(THF)][Al(NON^{Dipp})\{(OC(O)_2Te)\}]$ (**2**)



Crystallographic Details

Crystals were covered in inert oil and suitable single crystals were selected under a microscope and mounted on an Agilent SuperNova diffractometer fitted with an EOS S2 detector. Data were collected at 120 K (unless indicated otherwise) using focused microsource Cu K α radiation at 1.54184 Å. Intensities were corrected for Lorentz and polarisation effects and for absorption using multi-scan methods.^[S2] Space groups were determined from systematic absences and checked for higher symmetry. All structures were solved using direct methods with SHELXS,^[S3] refined on F^2 using all data by full matrix least-squares procedures with SHELXL-97,^[S4] within the WinGX^[S5] program. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in calculated positions or manually assigned from residual electron density where appropriate, unless otherwise stated. The functions minimized were $\Sigma w(F_2o - F_2c)$, with $w = [\sigma^2(F_2o) + aP^2 + bP]^{-1}$, where $P = [\max(F_2o)^2 + 2F_2c]/3$. The isotropic displacement parameters are 1.2 or 1.5 times the isotropic equivalent of their carrier atoms.

Additional Details:

K[Al(NON^{Dipp})(Te)(THF)] (K[1-Te·THF]): The THF solvate is disordered and was modelled with a methylene and the oxygen located over two positions. All atoms were refined isotropically.

[K(Et₂O)₃][Al(NON^{Dipp})(Te{¹³C(O)}₂)] (2): Data was collected at 150 K. The crystals contained extensive disorder in the coordinated Et₂O / THF molecules that also presents itself in the position of the tellurium atoms (that were each modelled over two positions). Although the coordinated Et₂O / THF were modelled as well as could be against the diffraction data obtained, a considerable number of constraints and restraints were required to give a satisfactory model. The data unequivocally shows the connectivity of the complex, but caution should be exercised when discussing any bond lengths and angles.

Computational Methods

DFT calculations were run with Gaussian 16 (A.03).^[S6] The Al, Si, Se and Te centres were described with the Stuttgart RECPs and associated basis sets,^[S7] and 6-31G** basis sets were used for all other atoms (BS1).^[S8] A polarization function was also added to Al ($\zeta_d = 0.190$) and Si ($\zeta_d = 0.284$), Se ($\zeta_d = 0.364$) and Te ($\zeta_d = 0.252$). Initial BP86^[S9] optimizations were performed using the 'grid = ultrafine' option, with all stationary points being fully characterized via analytical frequency calculations as either minima (all positive eigenvalues) or transition states (one negative eigenvalue). The Quantum Theory of Atoms in Molecules (QTAIM, AIMALL program^[S10]) and Natural Bonding Orbital (NBO3^[S11]) analyses were performed on the BP86-optimised geometries of the $[\text{Al}(\text{NON}^{\text{Dipp}})(\text{E})]^-$ anions.

Figure S12 Resonance forms contributing to the Al=E bond

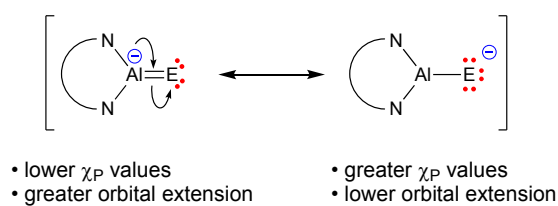
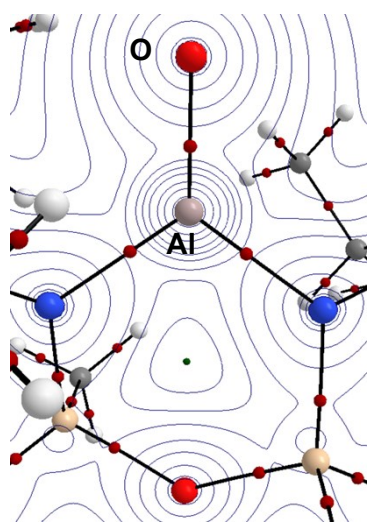
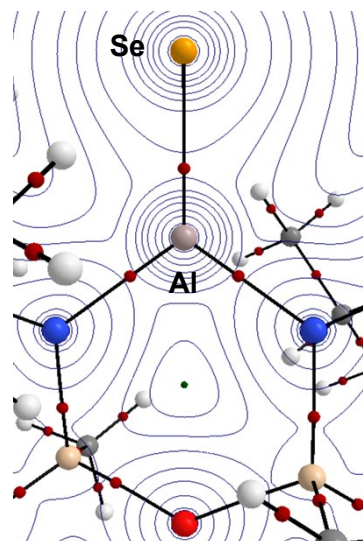


Figure S13 QTAIM molecular graph of the BP86-optimised geometry of the $[\text{Al}(\text{NON}^{\text{Dipp}})(\text{E})]^-$ anions. The electron density contours are computed in the $\{\text{Al}/\text{E}/\text{N}\}$ planes with bond critical points (BCPs) shown as small red spheres.

E = oxygen



E = selenium



E = tellurium

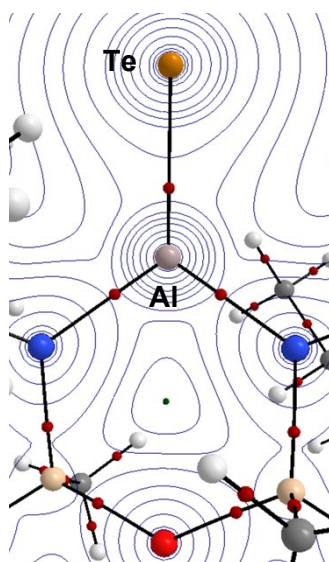


Table S1 Summary of DFT results for the anions [Al(NON^{Dipp})(E)]⁻

[Al(NON ^{Dipp})(E)] ⁻	E = O	E = Se	E = Te
Al–E / Å (X-ray)	1.6362(14) ^a	2.2032(6)	2.5039(7) ^b
Al–E / Å (computed)	1.66	2.24	2.46
% Difference: computed vs. X-ray bond length	+1.4	+1.6	–1.8
% Δd_{AlE}	6.5 ^c	6.6 ^d	3.4 ^e
$\Delta\chi_P^f$	1.83	0.94	0.49
NPA charges (<i>q</i>)	Al +1.93 O –1.23	Al +1.82 Se –1.23	Al +1.78 Te –1.19
$\Delta q = q(\text{Al}) - q(\text{E})$	3.16	3.05	2.97
Wiberg Bond Index (WBI)	1.01	1.07	1.09
Bond Critical Point (BCP) Analysis			
$\rho(r)^g$	0.115	0.068	0.061
$\nabla^2 \rho(r)^h$	+0.990	+0.183	+0.089
ε^i	0.033	0.108	0.139

a from [K{Al(NON^{Dipp})(O)}]₂; *b* from K[Al(NON^{Dipp})(Te)(THF)]; *c* using average $d(\text{Al-O}) = 1.74 \text{ \AA}$ from 35 \times Al-OH bonds; *d* using average $d(\text{Al-Se}) = 2.36 \text{ \AA}$ from 9 \times Al-SeH bonds; *e* using average $d(\text{Al-Te}) = 2.59 \text{ \AA}$ from 4 \times Al-TePh bonds; *f* $\Delta\chi_P = \chi_P(\text{E}) - \chi_P(\text{Al})$, where $\chi_P(\text{Al}) = 1.61$, $\chi_P(\text{O}) = 3.44$, $\chi_P(\text{Se}) = 2.55$, $\chi_P(\text{Te}) = 2.1$; *g* electron density associated with the BCP along the Al–E bond path ($\text{e}\text{\AA}^{-3}$); *h* Laplacian of the electron density ($\text{e}\text{\AA}^{-5}$); *i* ellipticities (ε).

Table S2 Molecular Orbital Coefficients for HOMO and HOMO–1 of K[Al(NON^{Dipp})(E)] (E = O, Se, Te)

Complex	Atom	Atomic Orbital	HOMO-1	HOMO
K[Al(NON ^{Dipp})(O)]	O	2 <i>p_x</i>	-0.32153	0.43893
		2 <i>p_y</i>	0.35718	0.33719
		2 <i>p_z</i>	-0.24282	0.04177
		3 <i>p_x</i>	-0.23005	0.31385
		3 <i>p_y</i>	0.26297	0.24063
		3 <i>p_z</i>	-0.16609	0.02241
	Al	4 <i>p_x</i>	-0.12337	0.10408
		4 <i>p_y</i>	0.00758	0.01487
		4 <i>p_z</i>	-0.09904	0.03581
K[Al(NON ^{Dipp})(Se)]	Se	3 <i>p_x</i>	0.46389	0.29125
		3 <i>p_y</i>	-0.19724	0.42146
		3 <i>p_z</i>	0.20287	-0.19510
		4 <i>p_x</i>	-0.33246	-0.20979
		4 <i>p_y</i>	-0.14881	-0.29935
		4 <i>p_z</i>	-0.13505	0.14318
	Al	3 <i>p_x</i>	0.07791	0.02196
		3 <i>p_y</i>	-0.06168	0.07524
		4 <i>p_z</i>	0.07005	0.00638
K[Al(NON ^{Dipp})(Te)]	Te	3 <i>p_x</i>	-0.05363	0.45839
		3 <i>p_y</i>	0.43911	0.05422
		4 <i>p_x</i>	-0.05107	0.45873
		4 <i>p_y</i>	0.44517	0.05602
		5 <i>p_x</i>	-0.01903	0.11185
		5 <i>p_y</i>	0.10200	0.00560
	Al	4 <i>p_x</i>	0.02520	-0.07428
		4 <i>p_y</i>	-0.15097	0.00216

NOTE: NBO Molecular Orbital Coefficients greater than ±0.07 are emphasised (in bold font).

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Cartesian Coordinates and Computed Energies
(in Hartrees)

[1-O]⁻

SCF (BP86) Energy = -1364.81348569

Enthalpy 0K = -1364.145631

Enthalpy 298K = -1364.100318

Free Energy 298K = -1364.222794

Lowest Frequency = 13.7467 cm⁻¹

Second Frequency = 16.7767 cm⁻¹

O 0.00007 -0.00029 -2.50696
Si -1.40748 -0.65413 1.97101
Si 1.40754 0.65395 1.97111
Al -0.00000 -0.00013 -0.84545
O -0.00010 0.00012 2.66607
N -1.50529 -0.15337 0.28378
N 1.50525 0.15331 0.28383
C -2.79762 0.04297 -0.31256
C -3.40993 1.33621 -0.27109
C -4.69011 1.51668 -0.82625
H -5.15518 2.50900 -0.79001
C -5.37492 0.45794 -1.43600
H -6.37336 0.61429 -1.86139
C -4.75710 -0.79473 -1.51837
H -5.27261 -1.61650 -2.02995
C -3.47811 -1.02561 -0.97437
C -2.64018 2.53691 0.27657
H -1.86360 2.13387 0.94972
C -3.50424 3.52665 1.08216
H -4.05209 3.01978 1.89570
H -2.86917 4.31063 1.53254
H -4.24854 4.04069 0.44661
C -1.91065 3.25702 -0.88365
H -2.64181 3.68858 -1.59171
H -1.27391 4.07841 -0.50526
H -1.27677 2.55477 -1.45570
C -2.81066 -2.38370 -1.18604
H -1.94364 -2.42114 -0.50460
C -3.73059 -3.57414 -0.84211
H -4.59248 -3.64254 -1.53116
H -3.17353 -4.52467 -0.92698
H -4.13168 -3.50215 0.18499
C -2.26234 -2.48558 -2.63049
H -1.52964 -1.67409 -2.82117
H -1.76291 -3.46121 -2.78397
H -3.08688 -2.40850 -3.36434
C -2.89066 -0.03148 2.98146
H -2.92599 1.06981 2.99953
H -3.84059 -0.39698 2.55718
H -2.81375 -0.39102 4.02232
C -1.27756 -2.53821 2.21615
H -1.11072 -2.77742 3.28132
H -2.19775 -3.05168 1.88808
H -0.43450 -2.95200 1.63737
C 1.27823 2.53804 2.21636
H 1.11213 2.77737 3.28163
H 2.19835 3.05125 1.88768
H 0.43492 2.95202 1.63808
C 2.89052 0.03068 2.98147
H 2.92470 -1.07064 3.00041
H 3.84060 0.39482 2.55634
H 2.81459 0.39117 4.02207

C 2.79756 -0.04288 -0.31259
C 3.47792 1.02581 -0.97437
C 4.75692 0.79512 -1.51840
H 5.27234 1.61697 -2.02994
C 5.37487 -0.45751 -1.43614
H 6.37333 -0.61371 -1.86156
C 4.69018 -1.51636 -0.82648
H 5.15533 -2.50864 -0.79035
C 3.40999 -1.33606 -0.27126
C 2.81027 2.38381 -1.18602
H 1.94321 2.42110 -0.50462
C 2.26203 2.48562 -2.63050
H 1.52949 1.67399 -2.82124
H 1.76242 3.46115 -2.78401
H 3.08663 2.40869 -3.36430
C 3.72998 3.57440 -0.84201
H 4.59192 3.64294 -1.53098
H 3.17277 4.52483 -0.92692
H 4.13100 3.50246 0.18513
C 2.64039 -2.53689 0.27631
H 1.86370 -2.13397 0.94941
C 1.91106 -3.25708 -0.88399
H 2.64235 -3.68851 -1.59201
H 1.27442 -4.07858 -0.50567
H 1.27712 -2.55491 -1.45608
C 3.50454 -3.52650 1.08197
H 4.05222 -3.01954 1.89556
H 2.86956 -4.31060 1.53228
H 4.24898 -4.04041 0.44648

[1-Se]⁻

SCF (BP86) Energy = -1299.02227563

Enthalpy OK = -1298.355901

Enthalpy 298K = -1298.309869

Free Energy 298K = -1298.434151

Lowest Frequency = 13.9919 cm⁻¹

Second Frequency = 23.8612 cm⁻¹

Se -0.00006 0.00040 -2.91602
Si -1.40147 -0.65558 2.14590
Si 1.40147 0.65515 2.14597
Al -0.00001 0.00011 -0.67263
O 0.00008 -0.00043 2.85005
N -1.50994 -0.12454 0.46044
N 1.50997 0.12448 0.46041
C -2.81464 0.16876 -0.07642
C -3.30626 1.51393 -0.05953
C -4.58549 1.79301 -0.57480
H -4.95029 2.82712 -0.56451
C -5.39664 0.78298 -1.10498
H -6.39127 1.01856 -1.50126
C -4.91221 -0.52829 -1.13478
H -5.53233 -1.32239 -1.56874
C -3.63633 -0.85843 -0.63627
C -2.44419 2.66706 0.45262
H -1.62265 2.21204 1.03285
C -3.20142 3.63285 1.38822
H -3.67731 3.09790 2.22842
H -2.50688 4.38245 1.80840
H -3.99421 4.18825 0.85457
C -1.81265 3.43574 -0.73261
H -2.59767 3.91463 -1.34644
H -1.13109 4.22862 -0.37191
H -1.24488 2.75750 -1.39491
C -3.16562 -2.30815 -0.75187
H -2.17650 -2.36498 -0.26749
C -4.11506 -3.28629 -0.02378
H -5.11443 -3.30607 -0.49604
H -3.71460 -4.31592 -0.05861
H -4.25831 -3.00899 1.03559
C -2.97960 -2.71915 -2.23017
H -2.25334 -2.05112 -2.72514
H -2.60567 -3.75766 -2.29823
H -3.93723 -2.66903 -2.78118
C -2.88834 -0.04972 3.15784
H -2.93689 1.05115 3.16766
H -3.83640 -0.42881 2.74176
H -2.80013 -0.40103 4.20053
C -1.24347 -2.53856 2.37561
H -1.00959 -2.76715 3.43035
H -2.17461 -3.06484 2.10761
H -0.43093 -2.94712 1.75169
C 1.24318 2.53805 2.37606
H 1.00931 2.76639 3.43085
H 2.17422 3.06452 2.10812
H 0.43056 2.94663 1.75225
C 2.88848 0.04932 3.15772
H 2.93724 -1.05155 3.16730
H 3.83648 0.42867 2.74171
H 2.80024 0.40038 4.20050
C 2.81465 -0.16878 -0.07649
C 3.63637 0.85850 -0.63616
C 4.91226 0.52843 -1.13469

H 5.53240 1.32259 -1.56849
C 5.39667 -0.78286 -1.10506
H 6.39131 -1.01838 -1.50134
C 4.58550 -1.79297 -0.57507
H 4.95030 -2.82708 -0.56491
C 3.30625 -1.51395 -0.05982
C 3.16570 2.30825 -0.75146
H 2.17665 2.36503 -0.26691
C 2.97948 2.71948 -2.22967
H 2.25319 2.05149 -2.72465
H 2.60548 3.75798 -2.29752
H 3.93704 2.66949 -2.78079
C 4.11528 3.28625 -0.02335
H 5.11458 3.30608 -0.49578
H 3.71483 4.31589 -0.05796
H 4.25869 3.00877 1.03594
C 2.44416 -2.66716 0.45213
H 1.62254 -2.21224 1.03232
C 1.81278 -3.43574 -0.73325
H 2.59789 -3.91451 -1.34706
H 1.13123 -4.22869 -0.37272
H 1.24504 -2.75745 -1.39554
C 3.20133 -3.63302 1.38771
H 3.67705 -3.09813 2.22806
H 2.50680 -4.38273 1.80769
H 3.99426 -4.18827 0.85411

[1-Te]⁻

SCF (BP86) Energy = -1297.75035738

Enthalpy OK = -1297.084115

Enthalpy 298K = -1297.037955

Free Energy 298K = -1297.162961

Lowest Frequency = 14.8142 cm⁻¹

Second Frequency = 22.7364 cm⁻¹

Te -0.00023 -0.00565 -2.95518
Si -1.39736 -0.65662 2.32137
Si 1.39772 0.66930 2.31741
Al 0.00011 -0.00069 -0.49506
O 0.00079 0.00714 3.02388
N -1.51245 -0.12098 0.63556
N 1.51289 0.12449 0.63460
C -2.81871 0.18640 0.10772
C -3.29179 1.53830 0.11668
C -4.56963 1.83110 -0.39464
H -4.91854 2.87080 -0.39195
C -5.39876 0.82865 -0.91026
H -6.39165 1.07519 -1.30404
C -4.93500 -0.49019 -0.92705
H -5.57075 -1.27983 -1.34613
C -3.66081 -0.83451 -0.43401
C -2.41988 2.68621 0.62402
H -1.58048 2.22479 1.17246
C -3.15755 3.62721 1.60041
H -3.60299 3.07242 2.44429
H -2.45799 4.37606 2.01358
H -3.97162 4.18311 1.10049
C -1.82728 3.48526 -0.56071
H -2.63148 3.97092 -1.14353
H -1.14277 4.27596 -0.20098
H -1.27144 2.82643 -1.25138
C -3.22304 -2.29658 -0.52354
H -2.21622 -2.35993 -0.07778
C -4.16508 -3.22639 0.27526
H -5.18210 -3.23527 -0.15799
H -3.79143 -4.26658 0.26105
H -4.26070 -2.90966 1.32882
C -3.10941 -2.76606 -1.99143
H -2.75571 -3.81282 -2.03487
H -4.08875 -2.72079 -2.50302
H -2.39588 -2.13255 -2.54610
C -2.88637 -0.06262 3.33623
H -2.93663 1.03797 3.35638
H -3.83335 -0.43931 2.91557
H -2.79848 -0.42356 4.37565
C -1.22460 -2.53845 2.54767
H -0.97114 -2.76303 3.59870
H -2.15700 -3.07060 2.29717
H -0.42067 -2.94402 1.91103
C 1.22279 2.55218 2.53296
H 0.96910 2.78267 3.58265
H 2.15470 3.08376 2.27936
H 0.41853 2.95329 1.89391
C 2.88768 0.08258 3.33506
H 2.93987 -1.01783 3.36010
H 3.83407 0.45899 2.91281
H 2.79907 0.44799 4.37285
C 2.81888 -0.18688 0.10856
C 3.66243 0.83051 -0.43748
C 4.93636 0.48238 -0.92851

H 5.57324 1.26933 -1.35091
C 5.39843 -0.83697 -0.90561
H 6.39114 -1.08655 -1.29794
C 4.56786 -1.83605 -0.38573
H 4.91546 -2.87616 -0.37819
C 3.29024 -1.53932 0.12386
C 3.22640 2.29268 -0.53369
H 2.21945 2.35908 -0.08867
C 3.11377 2.75571 -2.00371
H 2.39942 2.12074 -2.55564
H 2.76162 3.80279 -2.05197
H 4.09316 2.70668 -2.51487
C 4.16908 3.22496 0.26141
H 5.18646 3.23045 -0.17106
H 3.79683 4.26558 0.24202
H 4.26343 2.91308 1.31654
C 2.41674 -2.68373 0.63633
H 1.57742 -2.21862 1.18177
C 1.82417 -3.48819 -0.54475
H 2.62825 -3.97759 -1.12459
H 1.13863 -4.27638 -0.18148
H 1.26941 -2.83230 -1.23907
C 3.15272 -3.62041 1.61813
H 3.59780 -3.06172 2.45962
H 2.45217 -4.36659 2.03445
H 3.96682 -4.17946 1.12178