Electronic Supplemental Information

Soluble, Crystalline, and Thermally Stable Alkali CO_2^- and Carbonite (CO_2^{2-}) Clusters Supported by Cyclic(Alkyl)(Amino) Carbenes

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Experimental Procedures

General Considerations - All manipulations were carried out with the rigorous exclusion of air and moisture under an atmosphere of argon using standard Schlenk techniques or a MBRAUN LABmaster glovebox operating at <0.1 ppm H_2O and O_2 and equipped with a −39 °C freezer. All glassware used for experiments or measurements was oven-dried at 190 °C overnight before use. All reaction solvents were distilled over sodium/benzophenone and stored over 3 Å molecular seives. Deuterated acetonitrile was purchased from Cambridge Isotope Laboratories and purified by heating over calcium hydride for at least 48 h under followed by distillation under an argon atmosphere. NMR spectra were recorded at room temperature on a Bruker Avance 600 MHz (^{1}H: 600.13 MHz, ^{13}C: 150.90 MHz). Proton and carbon chemical shifts are reported in ppm and are referenced using the residual proton and carbon signals of the deuterated solvent (^{1}H; CD_3CN, δ 1.94, ^{13}C; CD_3CN, δ 1.32). Continuous wave (CW) EPR spectra were collected at room temperature using an X-band Bruker EMX spectrometer equipped with an ER 4123D dielectric resonator. Solid-state FTIR spectra were recorded on an Agilent Cary 630 FT-IR equipped with a diamond ATR unit in an argon-filled glovebox. Combustion microanalyses were performed using a PerkinElmer Series 2400 II CHNS/O Analyzer. Crystallographic data for **1**-**5** are summarized in Table S1. CO_2 used for the synthesis of **1** was purchased from Praxair (99.9% purity, part no. CD 3.0-T) and used as recieved without any further drying or purification. Diethyl-substituted cyclic (alkyl)(amino) carbene (CAAC) was prepared according to literature[1] and recrystallized from hexanes before use. In cases where alkali metals are used, shavings were taken off of commercially available metal ingots or rods by removing the oxidized outer layer and shaving the fresh surface as finely as possible with a blade.

*Synthesis of CAACCO₂ (**1**)* – Free diethyl CAAC (0.867 g, 2.77 mmol) was added to a 100 mL Schlenk tube and dissolved in a minimal amount of freshly dried THF (approx. 30 mL). The flask sidearm was attached directly to a mineral oil bubbler via flexible PVC tubing. A small gas sample bag was purged thoroughly with CO_2 before being filled with CO_2 fitted with a stainless-steel needle long enough to easily reach the solution. The needle was introduced through the septum of the Schlenk flask, the flask sidearm was opened, and CO_2 was allowed to bubble into the solution while maintaining steady positive pressure within the system (as indicated by the oil bubbler). Almost immediately after the introduction of the CO_2, a fine, bright-white precipitate was observed. Upon the depletion of the entire sample bag (approximately 5 min), the flask sidearm was closed, the needle was removed, and the flask connected to a Schlenk manifold. The white precipitate was isolated via cannula filtration, washed with dry hexanes (approx. 30 mL) and dried completely under reduced pressure. The remaining solids were collected yielding the product (0.800 g, 81%) as a highly pure white solid which is insoluble in non-polar hydrocarbon solvents, but increasingly soluble in THF, MeCN and CH_2Cl_2, respectively. Colorless, plate-like single crystals of the product suitable for X-ray diffraction were obtained by keeping a saturated THF solution of **1** at –39 °C. ^{1}H NMR: (600 MHz, CD_3CN) δ 1.13 (t, J = 7.3 Hz, 6H, $C(CH_2CH_3)_2$), 1.29 (t, J = 6 Hz, 12H, $CH(CH_3)_2$), 1.45 (s, 6H, $C(CH_3)_2$), 1.89 (m, 2H, $C(CH_2CH_3)_2$), 2.02 (m, 2H, $C(CH_2CH_3)_2$), 2.27 (s, 2H, backbone-CH_2), 2.80 (hept, J = 6.2 Hz, 2H, $CH(CH_3)_2$), 7.35 (d, J = 7.8 Hz, 2H, *meta*-H), 7.47 (t, J = 7.9 Hz, 1H, *para*-H); ^{13}C NMR (150.90 MHz, CD_3CN) δ 195.3, 159.2, 147.0, 131.5, 130.7, 126.6, 80.7, 57.5, 42.0, 32.2, 30.5, 29.5, 26.5, 24.6, 9.6; FTIR (solid state): ν 2968, 2925, 2874, 1664 (s), 1600 (m), 1470, 1353 (m), 1144, 1055 (w), 898 (w), 805 (s), 751 (m), 682 (w). Anal. Calc'd. for $C_{23}H_{35}NO_2$ (MW: 357.54 g mol^{-1}): C, 77.27; H, 9.87; N, 3.92; Found: 77.47, 10.11, 3.87. m.p.: 106 °C – 115 °C.

*Synthesis of $(THF)_3Li_2(CAACCO_2)_2$ **(2)*** – Compound **1** (150 mg, 0.420 mmol) was added to a 20 mL scintillation vial along with a stir bar and suspended in dry THF (approx. 15 mL). Freshly cut Li shavings (3.5 mg, 0.504 mmol) were added at RT and the resulting mixture was stirred vigorously for 36 h. The red-orange reaction mixture was filtered through a 0.45 μm PTFE syringe filter and the filtrate concentrated to a dark red oil under reduced pressure. The residue was dissolved in hexanes (approx. 3 mL) and stored in a -37 °C freezer yielding X-ray quality red block-like crystals after 2 days. After removal of supernatant, the crystals were dried under vacuum to yield **2** as paramagnetic crystalline red solids (103 mg, 52%). NOTE: This reaction is *highly* sensitive to the amount of reductant used. Precise control of the stoichiometry in this reaction is extremely important to ensure the successful isolation of pure product. EPR (CW, X-band) g = 1.99782 (a_{13C} = 2.24 G); FTIR (solid state): ν 2958, 2867, 1533 (s), 1341 (s), 1233 (s), 1196 (s), 1151(s), 1053 (s), 1053 (s), 911 (m), 798 (s), 742 (m). Anal. Calc'd. for $Li_2C_{58}H_{94}N_2O_7$ (MW: 945.28 g mol^{-1}): C, 73.70; H, 10.02; N, 2.96; Found: 73.07, 10.14, 3.02. m.p.: 73 °C – 82 °C.

*Synthesis of $(THF)_4Na_4(CAACCO_2)_4$ **(3)*** – Compound **1** (75 mg, 0.210 mmol) was added to a 20 mL scintillation vial along with a stir bar and dissolved in dry THF (approx. 8 mL). Sodium metal shavings (5.3 mg, 0.231 mmol) were added at RT, and the resulting mixture was stirred vigorously at RT for 16 h. The bright orange reaction mixture was filtered through a 0.45 μm PTFE syringe filter, and the resulting filtrate concentrated under reduced pressure until orange precipitate was observed. This precipitate was redissolved by agitation and gentle warming. The resulting saturated bright orange solution was kept at –39 °C to yield large, bright orange crystals of the product (43 mg, 45%). NOTE: This reaction is extremely sensitive to the amount of reductant used. Precise control of the stoichiometry in this reaction is extremely important to ensure the successful isolation of pure product. EPR (CW, X-band) g = 1.99782 (a_{13C} = 2.24 G); FTIR (solid state): ν 2964, 2867, 1517 (s), 1465 (m), 1297 (m), 1222 (m), 1055 (s), 902 (m), 798 (m), 743 (m); Anal. Calc'd for $NaC_{27}H_{43}NO_3$ (MW: 452.63 g mol^{-1}): C, 71.65; H, 9.58; N, 3.09; Found: C, 71.14; H, 9.91; N, 2.92. m.p.: 74 °C – 80 °C.

*Synthesis of $(THF)_4K_4(CAACCO_2)_4$ **(4)*** – Compound **1** (75 mg, 0.210 mmol) was added to a 20 mL scintillation vial along with a stir bar and dissolved in dry THF (approx. 8 mL). KC_8 flakes (34 mg, 0.252 mmol) were added at RT, and the resulting mixture was stirred vigorously for 36 h. The purple-red mixture was filtered through a 0.45 μm PTFE syringe filter and concentrated to *ca.* 3 mL under reduced pressure. Hexanes (approx. 1 mL) were added and the mixture subsequently filtered. Red block-like crystals suitable for X-ray diffraction studies were obtained from keeping the filtrate at RT. The supernatant was stored at -37 °C yielding a second crop of crystals which were recovered after 3 days and dried under vacuum (total isolated yield: 84 mg, 85%). NOTE: This reaction is extremely sensitive to the amount of reductant used. Precise control of the stoichiometry in this reaction is extremely important to ensure the successful isolation of pure product. FTIR (solid state): ν 2958, 2863, 1517 (s), 1463 (m), 1297 (s), 1226 (s), 1153 (m), 1055 (m), 926 (w), 798 (m), 742 (m). Satisfactory elemental analysis results could not be obtained for this compound. m.p.: 94 °C – 99 °C.

*Synthesis of $(THF)_nLi_2(CAACCO_2)$ $0<n<0.333$ [**5** ($n=0.333$) and **6** ($n=0.0$)]* – Compound **1** (100 mg, 0.280 mmol) was added to a Schlenk tube along with a stir bar and dissolved in dry THF (approx. 20 mL). Lithium metal shavings (7.8 mg, 1.12 mmol) were added at RT, and the resulting mixture was stirred vigorously at RT for 3 d, yielding a deep red/orange solution. The reaction mixture was dried to a sticky residue under reduced pressure, extracted with toluene (10 mL) and filtered. The deep red/orange extract was dried completely under reduced pressure and triturated twice with hexanes (2 x 4 mL) to yield a deep red/orange glassy solid which was collected and confirmed to be an inseperable mixture of **5** and **6**. This mixture apparently results from the incomplete removal of THF from the molecular structure of the product. This mixture can be accurately described as one species with the general formula $(THF)_nLi_2(CAACCO_2)$ $0<n<0.333$ with a molar mass between 371.422 g/mol ($n = 0$) and 395.456 g/mol ($n = 0.333$). The true amount of THF (value of n) in this bulk sample was analyzed by elemental analysis. The results of this analysis gave an experimental CHN content closer to the expected values for $(THF)_{0.333}Li_2(CAACCO_2)$ (77 mg, 70 %). FTIR (solid state): ν 2960, 2930, 2865, 1679 (m), 1599 (s), 1467 (s), 1438 (s), 1381 (s), 1250 (s), 1176 (s), 1129 (s), 1051 (s), 803 (s), 754 (s); Anal. Calc'd for $C_{76}H_{113}Li_6N_3O_8$ (MW: 1238.26 g mol^{-1}): C, 73.49; H, 9.69; N, 3.34; Found: C, 72.06; H, 9.77; N, 3.53; m.p.: 118 °C – 125 °C.

*Synthesis of $Na_{12}(CAACCO_2)_6$ (**7**)* – Compound **1** (100 mg, 0.280 mmol) was added to a Schlenk tube along with a stir bar and dissolved in dry THF (approx. 20 mL). Sodium metal shavings (26 mg, 1.12 mmol) were added, and the resulting mixture was stirred vigorously for 16 h, yielding a dark orange solution. The reaction mixture was dried completely under reduced pressure and extracted with hexane (15 mL). The filtrate was dried completely under vacuum to yield the product as a dark orange crystalline solid. A saturated hexane solution of the product was kept at –39 °C to yield orange plate-like crystals of the product suitable for X-ray diffraction (97 mg, 86%). NOTE: This reaction can also be performed successfully using a 5% sodium dispersion on sodium chloride (5 wt. % Na/NaCl) reported by Jones *et al.*[2] in place of sodium shavings. FTIR (solid state): ν 2956, 2923, 2865, 1584 (m), 1433 (s), 1246 (s), 1120 (s), 1062 (s), 799 (m), 753 (m). Anal. Calc'd for $Na_2C_{23}H_{35}NO_2$ (MW: 403.52 g mol^{-1}): C, 68.46; H, 8.74; N, 3.47; Found: C, 68.16; H, 8.74; N, 3.22; m.p.: decomposition at 151 °C.

*Synthesis of $K_{10}(CAACCO_2)_5$ (**8**)* – Compound **1** (100 mg, 0.280 mmol) was added to a Schlenk tube along with a stir bar and dissolved in dry THF (approx. 20 mL). Potassium metal shavings (33 mg, 0.836 mmol) were added, and the resulting mixture was stirred vigorously for 6 h, yielding a dark red-purple solution. The reaction mixture was dried completely under reduced pressure and extracted with hexane (15 mL). The filtrate was dried completely under vacuum to yield the product as a dark red-purple crystalline solid. A saturated hexane solution of the product was kept at –39 °C to yield dark red-purple plate-like crystals of the product suitable for X-ray diffraction (116 mg, 96%). NOTE: This reaction can also be performed successfully using potassium graphite (KC_8) in place of potassium shavings with comparable yields. FTIR (solid state): ν 2956, 2927, 2863, 1502 (m), 1461 (m), 1431 (m), 1246 (s), 1062 (s), 796 (m), 751 (m); Anal. Calc'd for $K_2C_{23}H_{35}NO_2$ (MW: 435.73 g mol^{-1}): C, 63.40; H, 8.10; N, 3.21; Found: C, 62.90; H, 8.59; N, 2.94; m.p.: 162 °C – 171 °C.

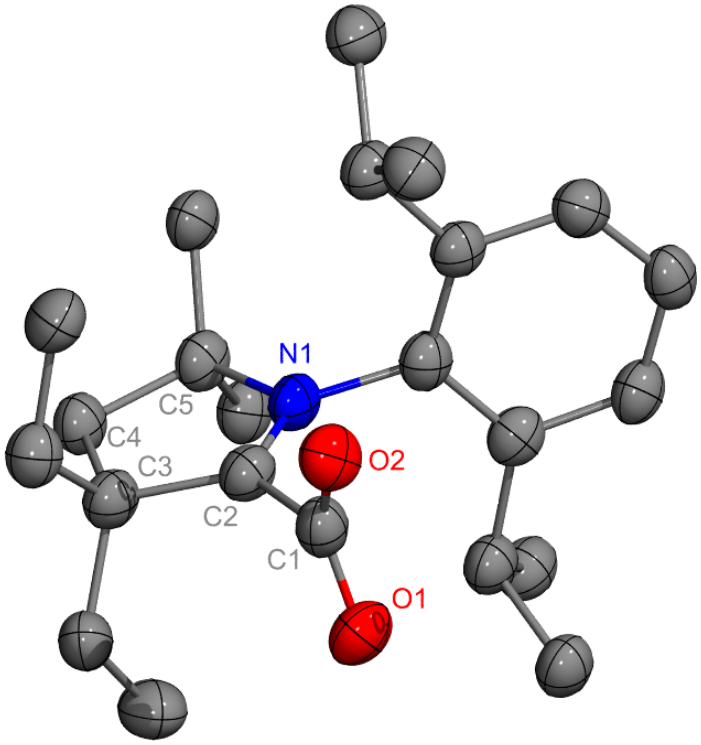


Figure S1. Molecular Structure of **1** (thermal ellipsoids set at 50% probability, H atoms omitted for clarity).

NMR Spectra

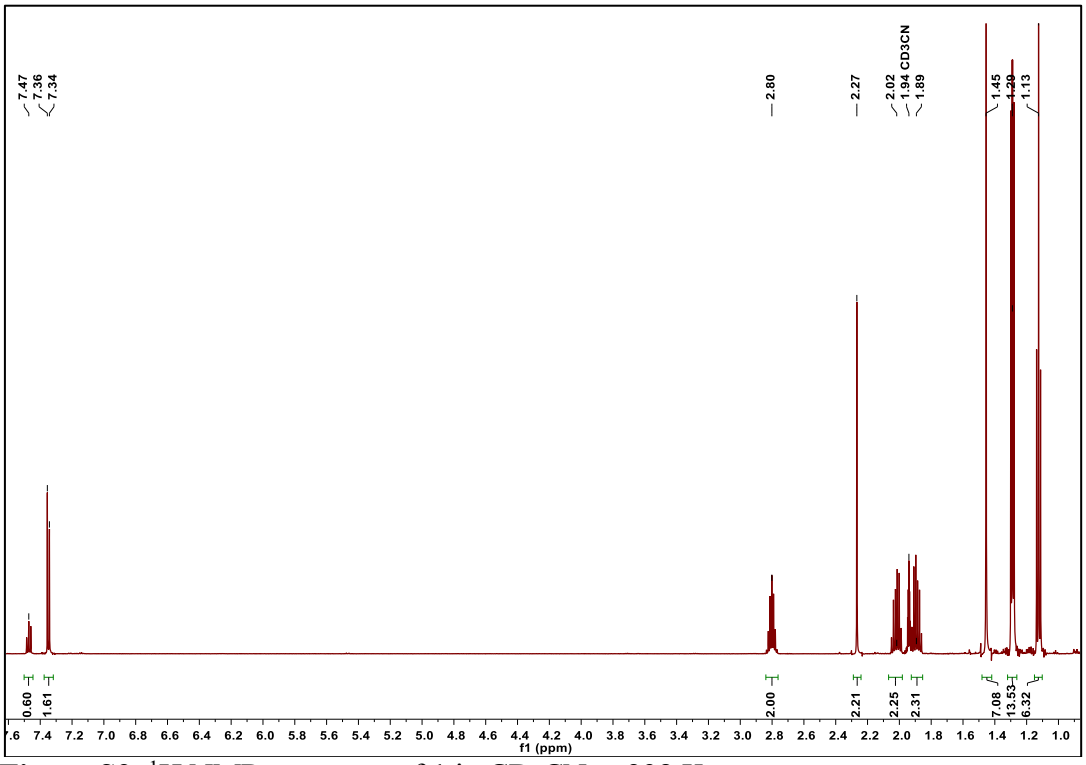


Figure S2. ^{1}H NMR spectrum of **1** in CD_3CN at 298 K.

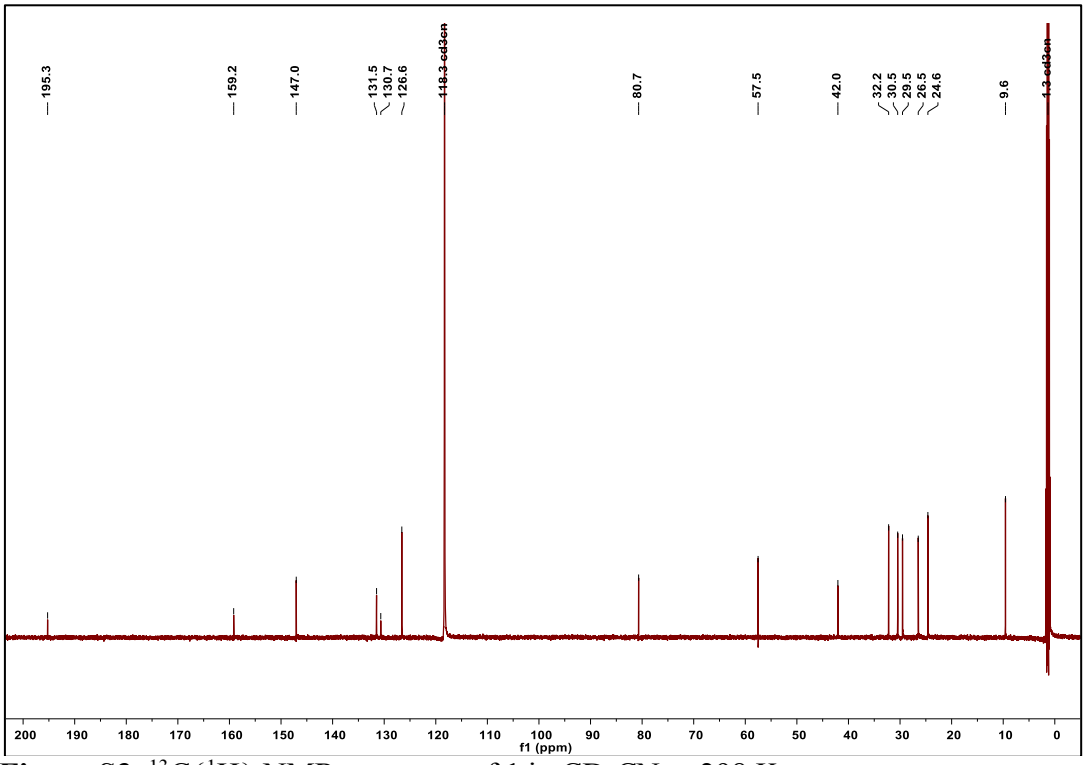


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in CD_3CN at 298 K.

FTIR Spectra

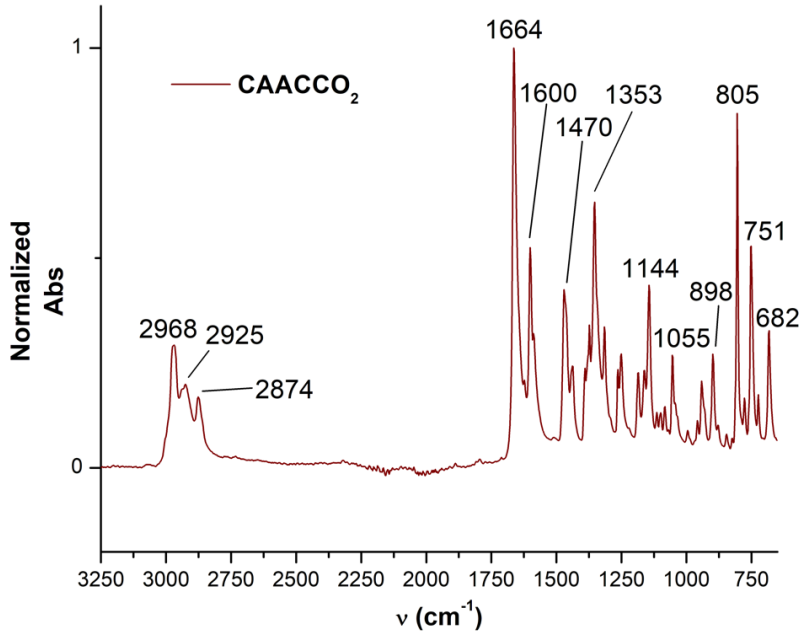


Figure S4. FTIR (solid state) of **1** at 298 K.

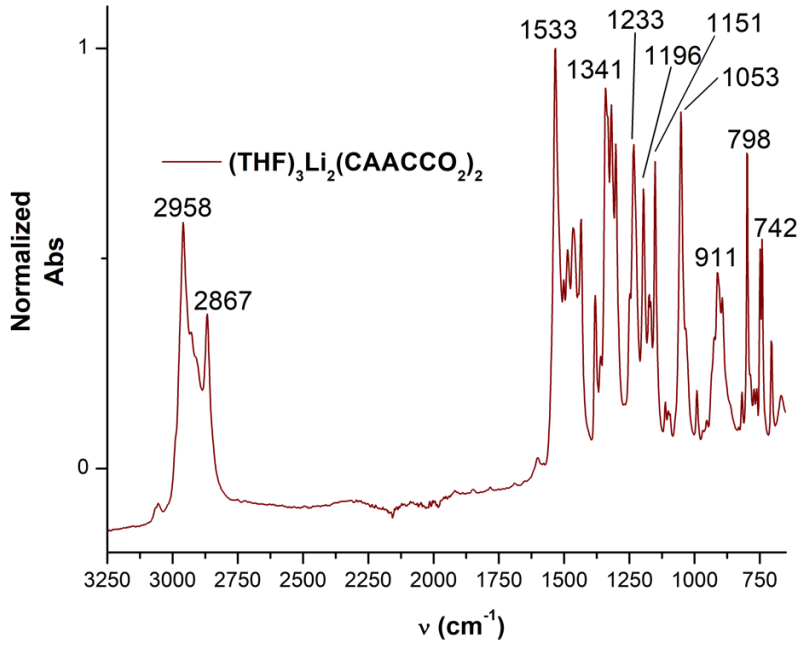


Figure S5. FTIR (solid state) of **2** at 298 K.

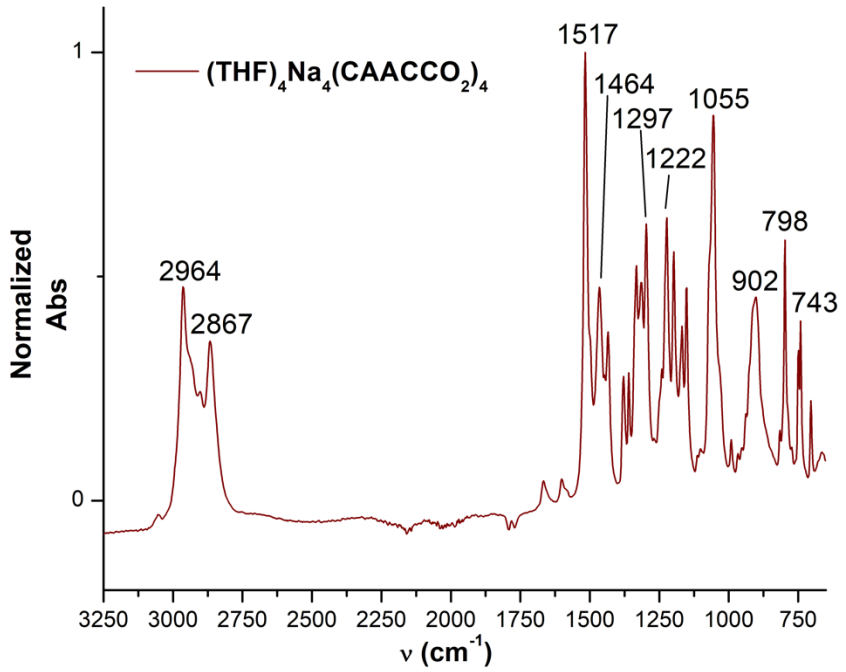


Figure S6. FTIR (solid state) of **3** at 298 K.

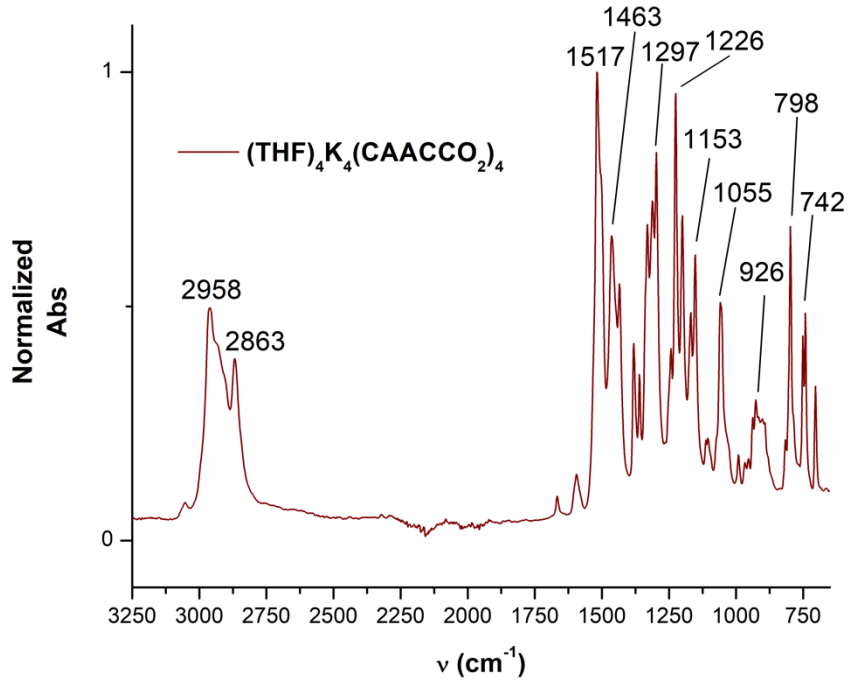


Figure S7. FTIR (solid state) of **4** at 298 K.

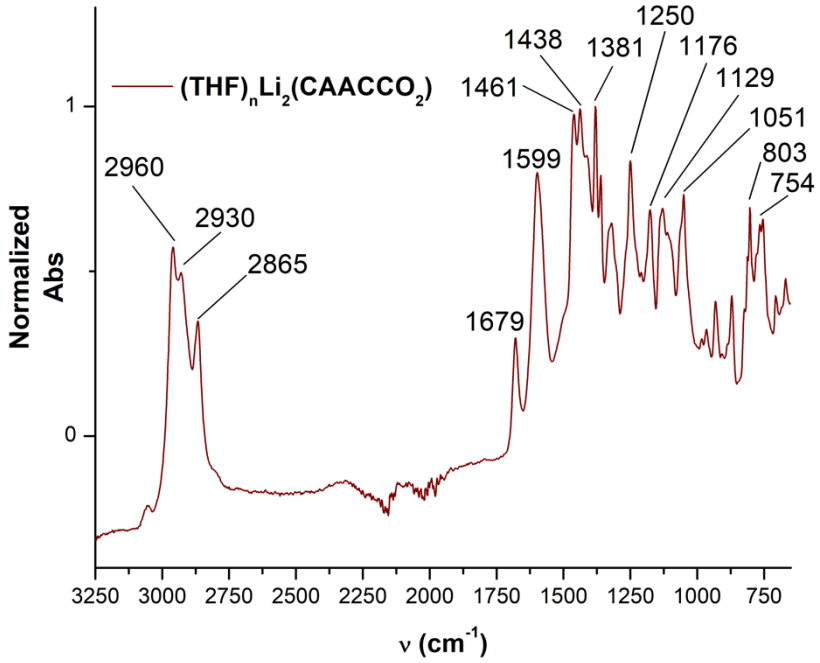


Figure S8. FTIR (solid state) of mixture of **5** (n=0.333) and **6** (n=0.0**)** at 298 K.

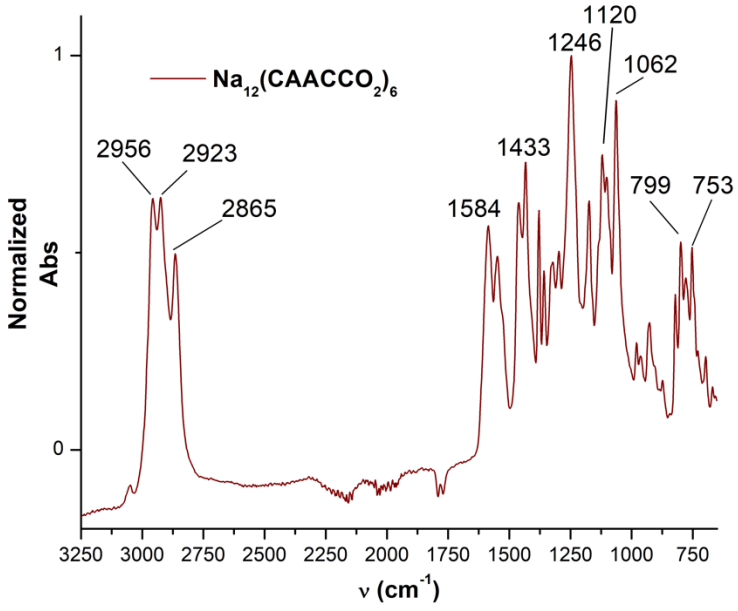


Figure S9. FTIR (solid state) of **7** at 298 K.

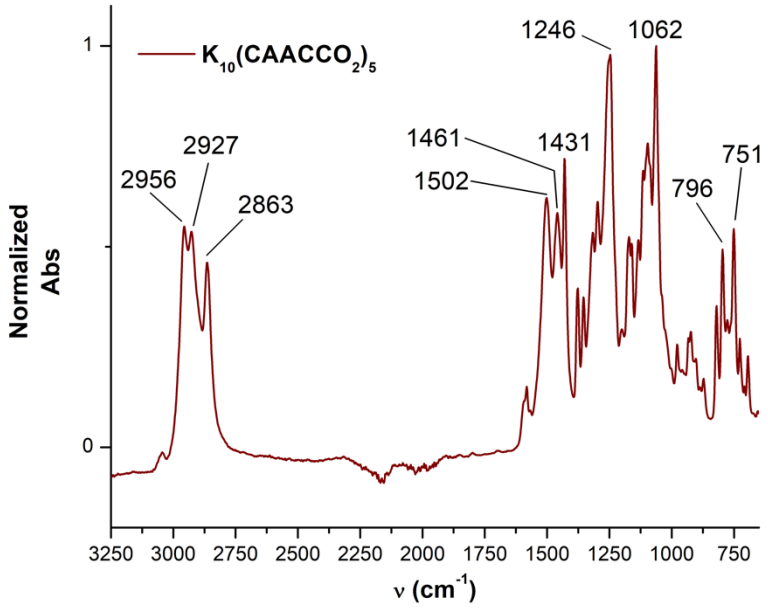


Figure S10. FTIR (solid state) of **8** at 298 K.

Electronic Absorption (UV/Vis) Spectra

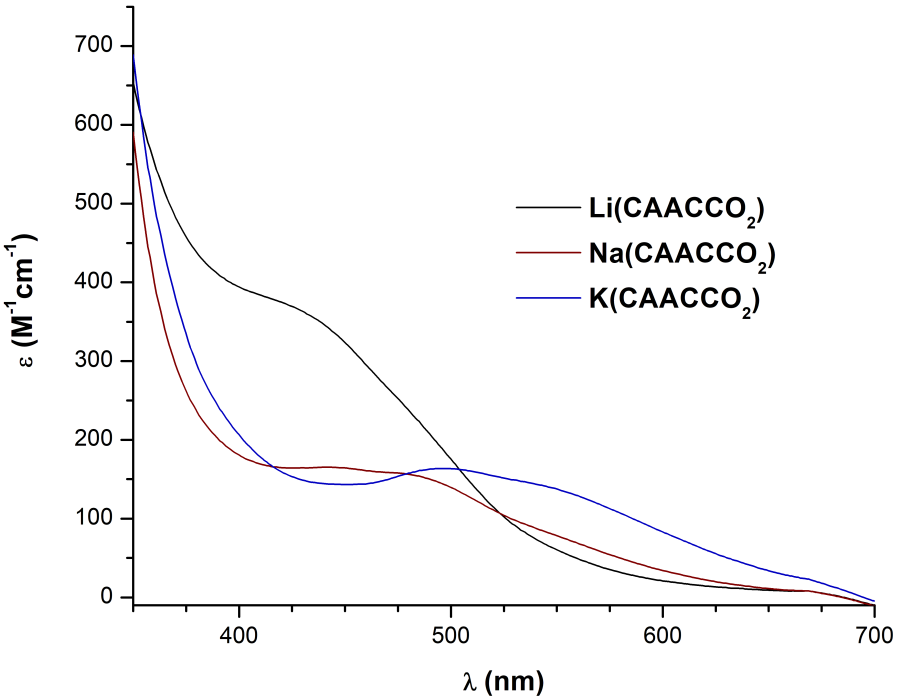


Figure S11. Stacked electronic absorption spectra of compounds **2-4** in toluene (0.5 mg/mL).

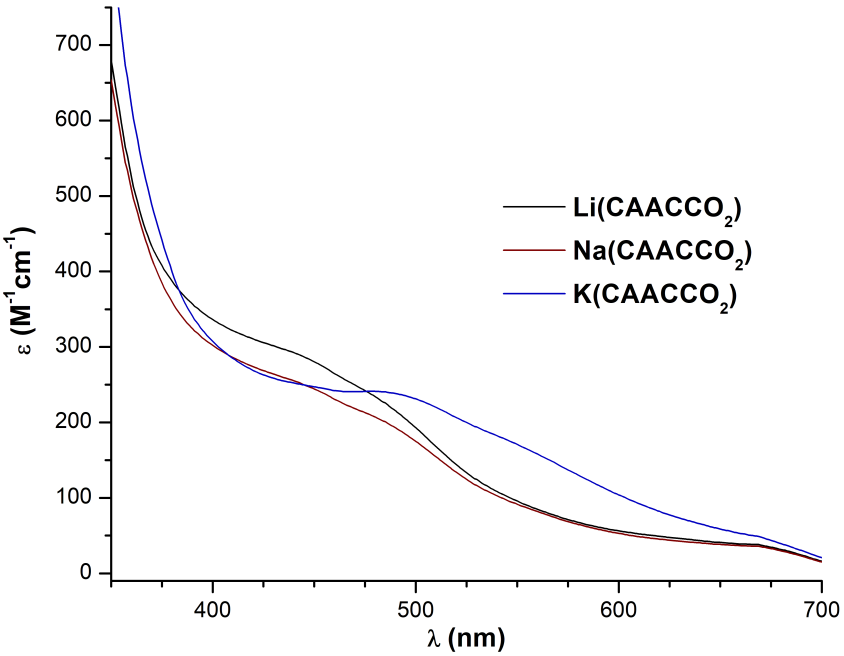


Figure S12. Stacked electronic absorption spectra of compounds **2-4** in THF (0.5 mg/mL).

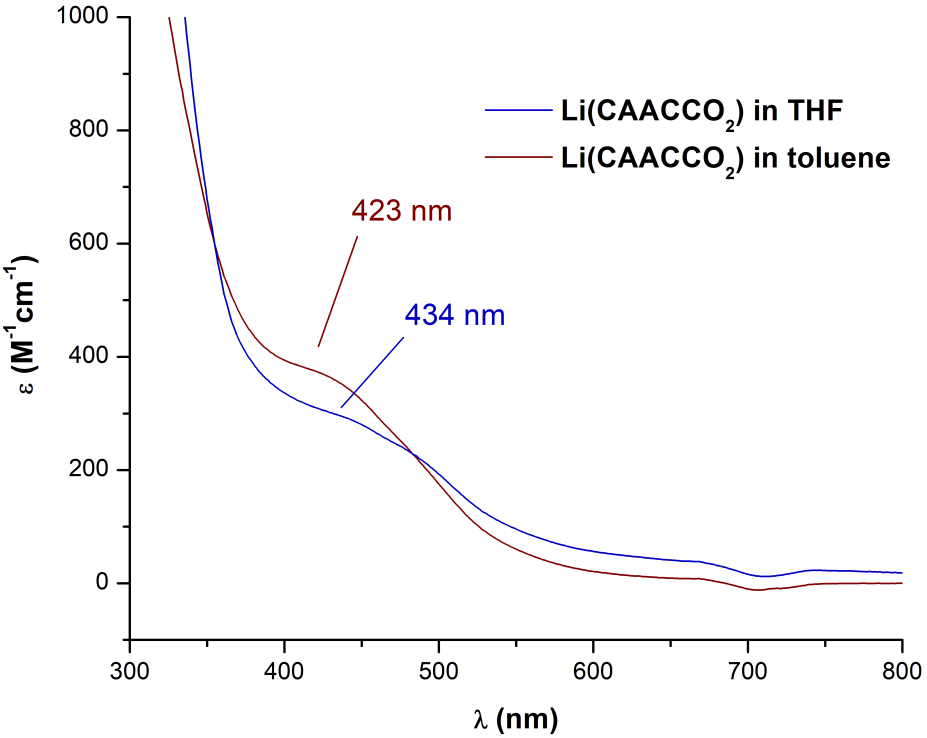


Figure S13. Stacked electronic absorption spectra of **2** in toluene and THF (0.5 mg/mL).

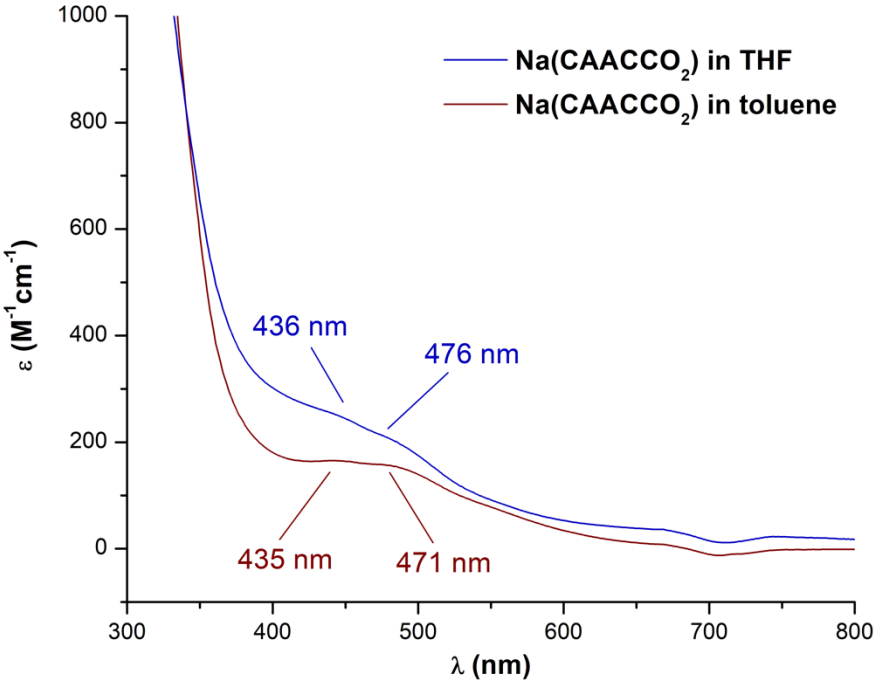


Figure S14. Stacked electronic absorption spectra of **3** in toluene and THF (0.5 mg/mL).

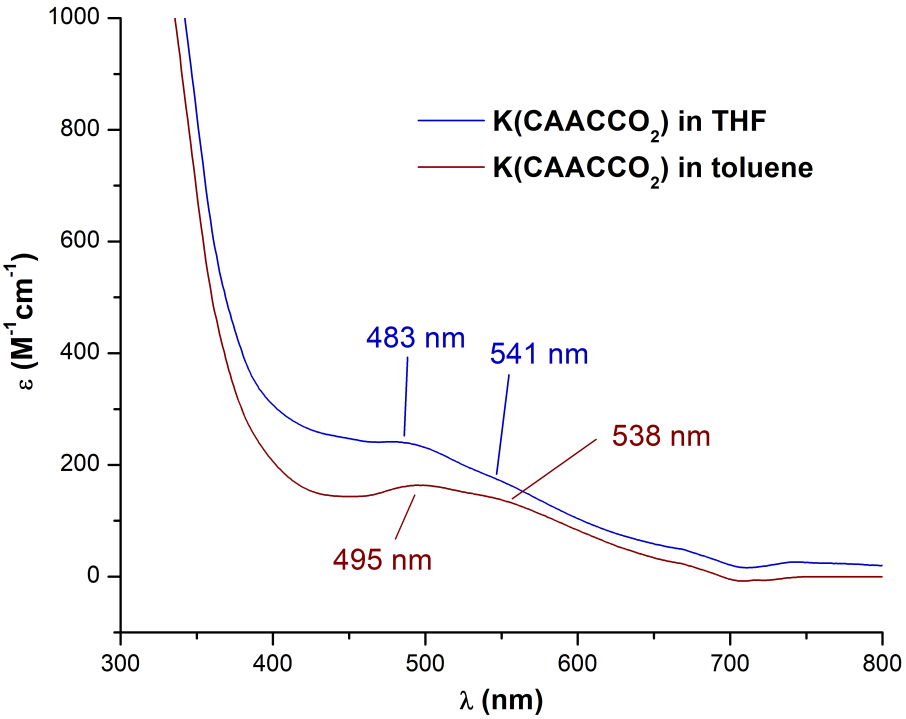


Figure S15. Stacked electronic absorption spectra of **4** in toluene and THF (0.5 mg/mL).

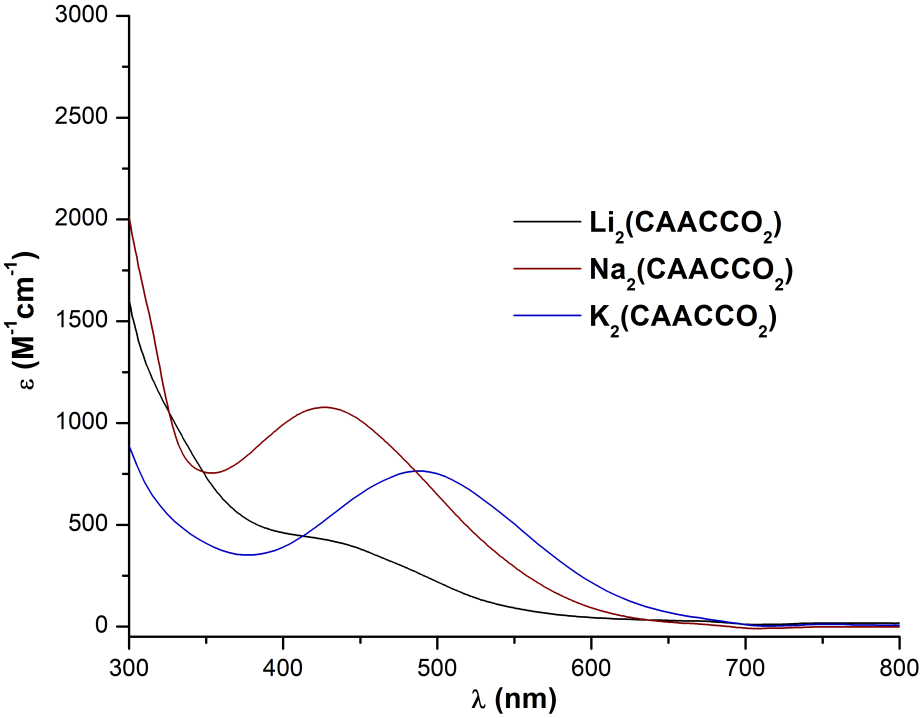


Figure S16. Stacked electronic absorption spectra of compounds **5-8** in toluene (0.5 mg/mL).

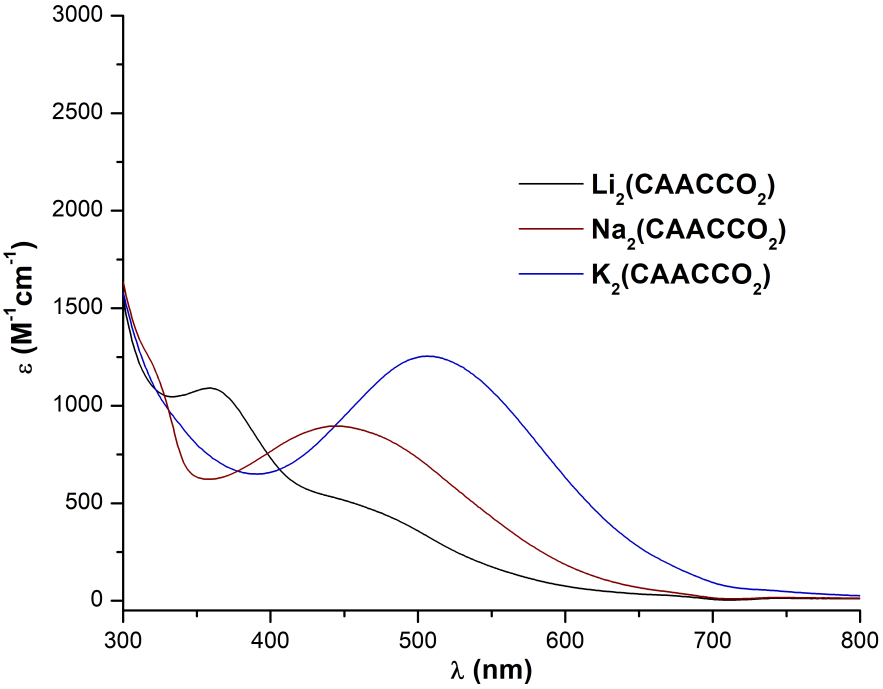


Figure S17. Stacked electronic absorption spectra of compounds **5-8** in THF (0.5 mg/mL).

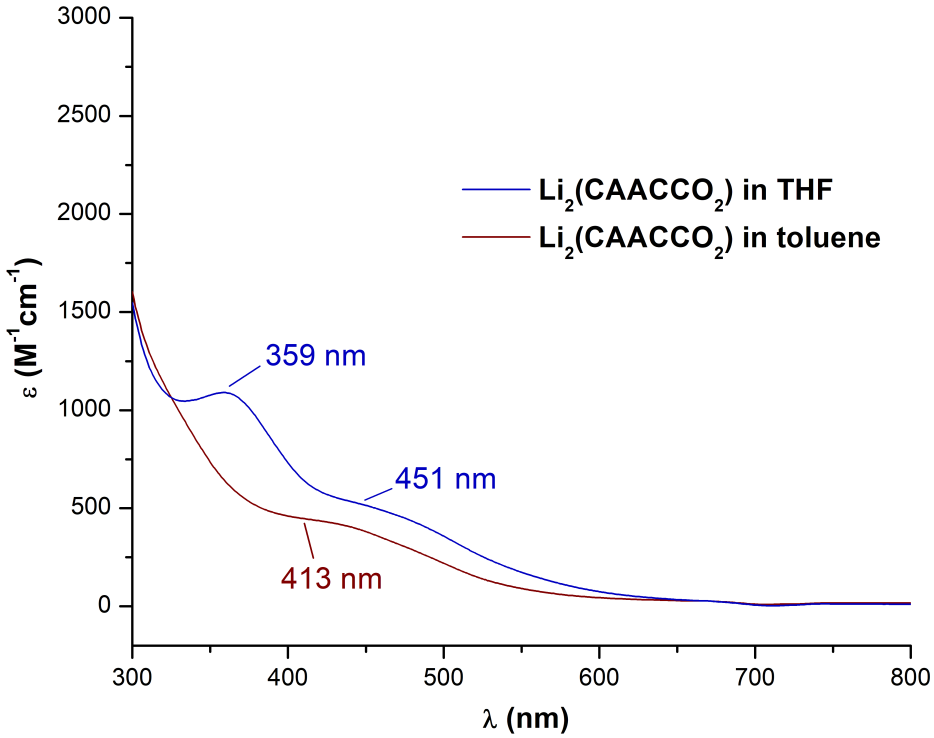


Figure S18. Stacked electronic absorption spectra of **5/6** in toluene and THF (0.5 mg/mL).

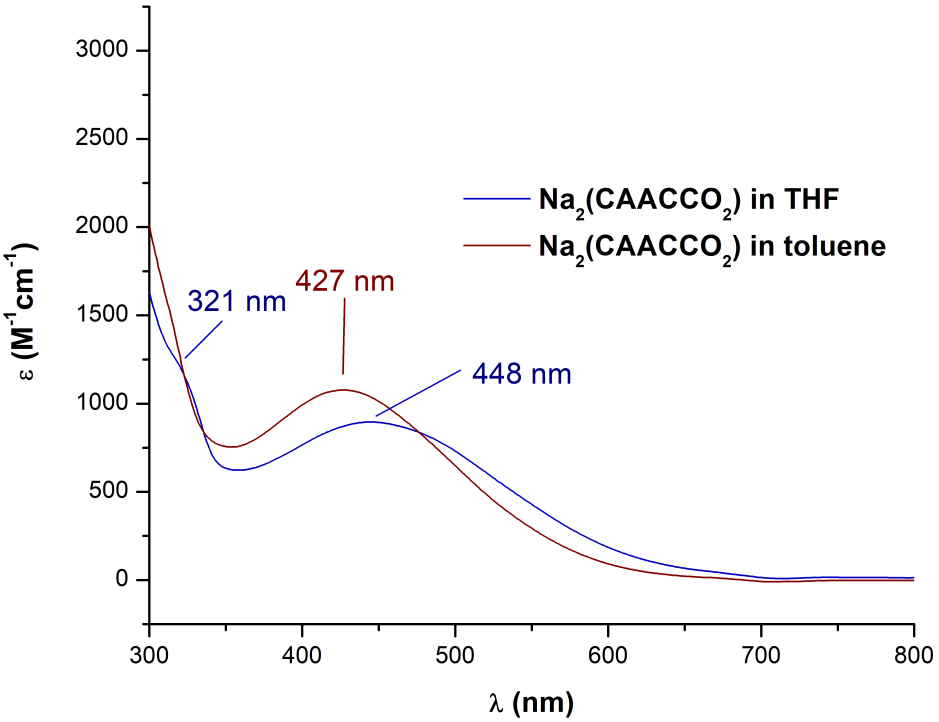


Figure S19. Stacked electronic absorption spectra of **7** in toluene and THF (0.5 mg/mL).

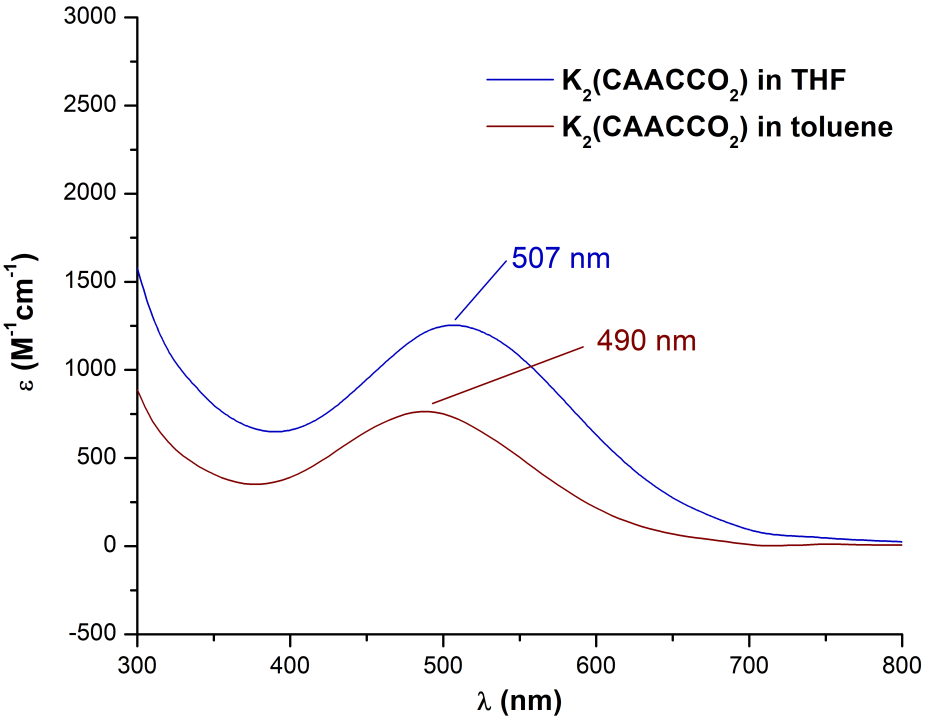


Figure S20. Stacked electronic absorption spectra of **8** in toluene and THF (0.5 mg/mL).

EPR Spectra

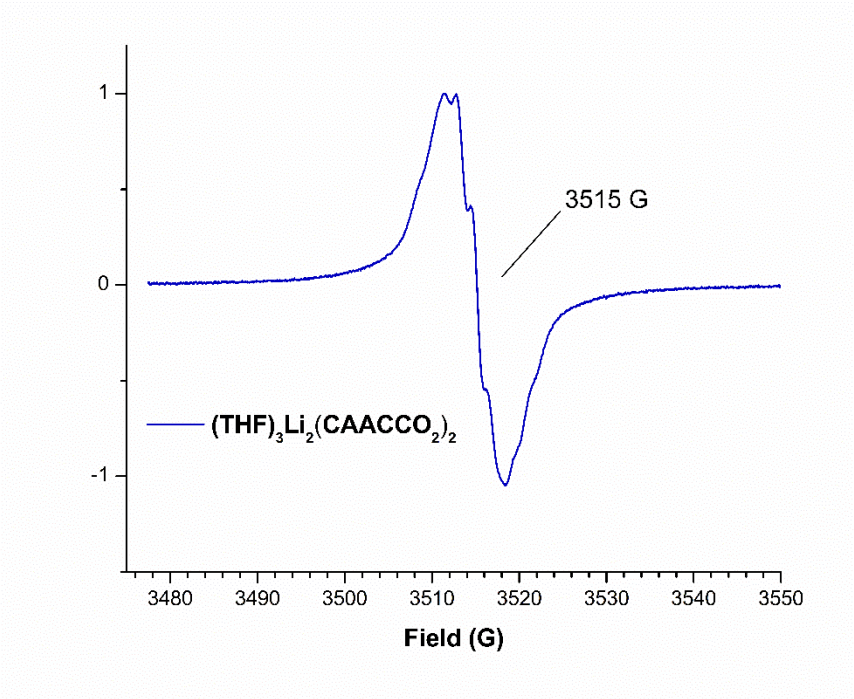


Figure S21. EPR spectrum of **2** in toluene solution at 298 K.

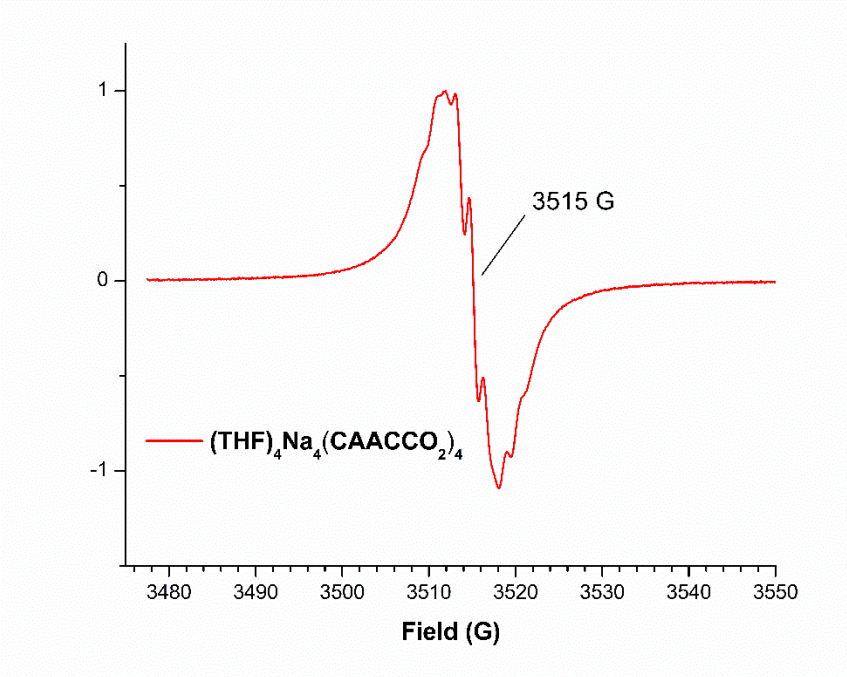


Figure S22. EPR spectrum of **3** in toluene solution at 298 K.

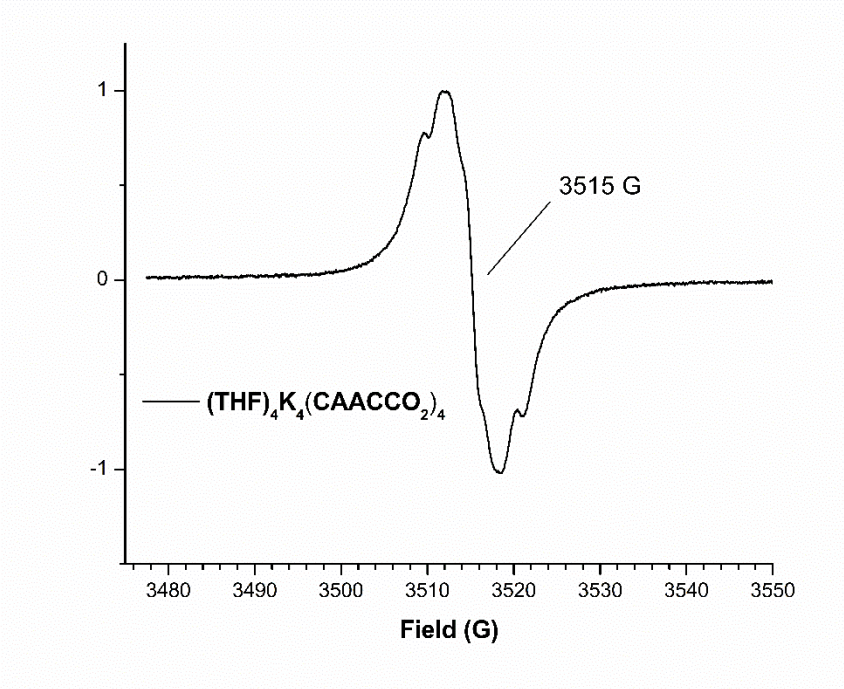


Figure S23. EPR spectrum of **4** in toluene solution at 298 K.

Crystallographic Refinement Details

A suitable single crystal of **1-8** was coated with Paratone oil and mounted on a MiTeGen MicroLoop.The X-ray intensity data were measured on a Bruker Kappa APEXII Duo system with a Incoatec Microfocus IμS (Cu K_α, $\lambda = 1.54178$ Å) and a multi-layer mirror monochromator (**1, 3, 4, 6-8**) or a fine-focus sealed tube (Mo K_α, $\lambda = 0.71073$ Å) and a graphite monochromator (**2, 5**). The frames were integrated with the Bruker SAINT software package[2] using a narrow-frame algorithm. Data were corrected for absorption effects using the Multi-Scan method (SADABS or TWINABS).[3] Each structure was solved and refined using the Bruker SHELXTL Software Software Package[4] within APEX3[3] and OLEX2.[5] Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in geometrically calculated positions with $U_{iso} = 1.2U_{equiv}$ of the parent atom ($1.5U_{equiv}$ for methyl).

Compound **1** was identified as a two-component twin using CELL_NOW.[6] Starting with 633 reflections, 471 reflections were fit to the first domain, 437 to the second domain (160 exclusively), with 2 unindexed reflection remaining. The twin domain was oriented at a 179.9º rotation about the reciprocal axis 0.001 0.001 1.000. The twin law was -1.000 -0.001 0.001 / 0.004 -1.000 0.002 / 0.527 0.001 1.000. It was refined as a two-component twin on HKLF5 data, with the BASF for the twin domains refining to 0.40601.

In compound **3**, THF solvent located in the crystal lattice was severely disordered and could not be adequately modeled with or without restraints. Thus, the structure factors were modified using the PLATON SQUEEZE technique,[7] in order to produce a "solvate-free" structure factor set. PLATON reported a total electron density of 713 e^- and total solvent accessible volume of 3366 $Å^3$.

In compound **4**, three carbon atoms of the coordinated THF solvent were found to be disordered over two positions. The relative occupancy of the two conformations was freely refined, and no constraints or restraints were needed. The hexane solvent was refined at reduced occupancy with constraints on its anisotropic displacement parameters and restraints on its bonds to account for its location near the three-fold axis.

In compound **5**, hexane solvent located in the crystal lattice was severely disordered and could not be adequately modeled with or without restraints. Thus, the structure factors were modified using the PLATON SQUEEZE technique,[7] in order to produce a "solvate-free" structure factor set. PLATON reported a total electron density of 120 e^- and total solvent accessible volume of 537 $Å^3$. One methylene group of a coordinated THF was disordered over two positions. The relative occupancy was freely refined, with constraints on the anisotropic displacement parameters of the disordered atoms.

In compound **6**, several lithium atoms and part of one ligand were disordered over two positions. The relative occupancies were freely refined. Constraints and restraints were used on anisotropic displacement parameters and bond lengths of the disordered ligand. No constraints or restraints were needed on the disordered lithium atoms. Solvent located in the crystal lattice was severely disordered and could not be adequately modeled with or without restraints. Thus, the structure factors were modified using the PLATON SQUEEZE technique,[7] in order to produce a "solvate-free" structure factor set. PLATON reported a total electron density of 418 e^- and total solvent accessible volume of 2012 $Å^3$.

Compound 8 was identified as a two-component twin using the TWINROTMAT feature of Platon.[8] It found a 180° rotation around the (1 0 0) axis. The twin law was 1.000 0.000 0.000 / 0.000 -1.000 0.000 / 0.000 0.000 -1.000, and the BASF refined to 0.2394.

Table S1. Crystallographic details for compounds **1-8**.

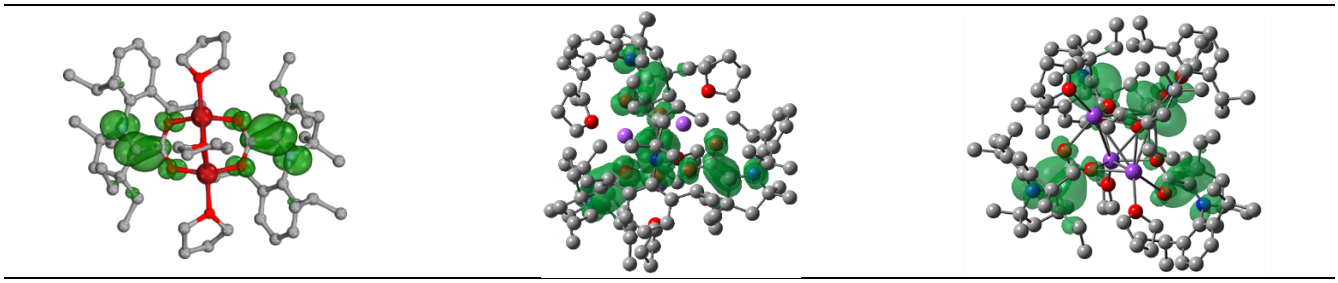
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
CCDC number	1991606	1991607	1991608	1991609	1991611	1991610	1991612	1991613
Formula	$C_{27}H_{43}NO_3$	$C_{58}H_{94}Li_2N_2O_7$	$C_{108}H_{172}N_4Na_4O_{12}$	$C_{116}H_{190.67}K_4N_4O_{12}$	$C_{77}H_{121}Li_6N_3O_8$	$C_{138}H_{210}Li_{12}N_6O_{12}$	$C_{144}H_{224}N_6Na_{12}O_{12}$	$C_{115}H_{175}K_{10}N_5O_{10}$
FW (g/mol)	429.62	945.23	1810.45	1989.78	1258.40	2228.39	2507.16	2178.59
Temp (K)	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)
λ (Å)	1.54178	0.71073	1.54178	1.54178	0.71073	1.54178	1.54178	1.54178
Size (mm)	0.048 x 0.065 x 0.256	0.418 x 0.489 x 0.629	0.051 x 0.090 x 0.100	0.071 x 0.101 x 0.112	0.148 x 0.262 x 0.430	0.096 x 0.204 x 0.208	0.080 x 0.102 x 0.233	0.138 x 0.138 x 0.187
Crystal habit	colorless plate	red block	orange block	orange block	red block	yellow plate	orange plate	red plate
Crystal system	monoclinic	monoclinic	cubic	cubic	monoclinic	triclinic	monoclinic	monoclinic
Space group	P 2_1/c	C 2/c	I -4 3 d	I -4 3 d	P 2_1	P -1	P 2_1/n	P 2_1/c
a (Å)	8.2116(4)	16.8366(18)	32.0084(5)	32.4579(6)	14.2409(17)	15.9758(15)	16.2060(5)	25.5103(18)
b(Å)	14.8475(7)	13.6239(15)	32.0084(5)	32.4579(6)	14.1749(17)	16.9105(15)	29.7416(9)	27.8549(17)
c (Å)	20.2921(9)	24.398(3)	32.0084(5)	32.4579(6)	20.804(2)	29.646(3)	30.0188(8)	16.3237(11)
α (°)	90	90	90	90	90	84.635(6)	90	90
β (°)	96.280(4)	91.454(2)	90	90	104.449(4)	79.342(6)	102.473(2)	90.336(5)
γ (°)	90	90	90	90	90	87.435(6)	90	γ = 90
Volume (Å^3)	2459.2(2)	5594.6(10)	32793.8(15)	34194.9(19)	4066.7(8)	7833.4(13)	14127.3(7)	11599.2(13)
Z	4	4	12	12	2	2	4	4
Density (g/cm^3)	1.160	1.122	1.100	1.160	1.028	0.945	1.179	1.248
μ (mm^{-1})	0.576	0.071	0.685	1.842	0.064	0.442	0.891	3.737
θ range (°)	3.70 to 68.39	1.67 to 29.13	3.38 to 68.28	3.33 to 68.28	1.01 to 25.76	1.52 to 68.52	2.12 to 68.36	1.59 to 66.59
Index ranges	-9 ⩽ h ⩽ 9 0 ⩽ k ⩽ 17 0 ⩽ l ⩽ 24	-23 ⩽ h ⩽ 22 -18 ⩽ k ⩽ 18 -33 ⩽ l ⩽ 33	-33 ⩽ h ⩽ 30 -38 ⩽ k ⩽ 30 -38 ⩽ l ⩽ 38	-39 ⩽ h ⩽ 35 -36 ⩽ k ⩽ 38 -39 ⩽ l ⩽ 29	-17 ⩽ h ⩽ 15 -17 ⩽ k ⩽ 15 -25 ⩽ l ⩽ 25	-19 ⩽ h ⩽ 19 -20 ⩽ k ⩽ 20 -34 ⩽ l ⩽ 35	-19 ⩽ h ⩽ 10 -35 ⩽ k ⩽ 35 -36 ⩽ l ⩽ 30	-30 ⩽ h ⩽ 30 -33 ⩽ k ⩽ 24 -19 ⩽ l ⩽ 19
Reflns collected	30686	31936	42456	43247	58000	115172	107931	87204
Independent reflns	4553 [R_{int} = 0.2324]	7529 [R_{int} = 0.0284]	5015 [R_{int} = 0.0862]	5244 [R_{int} = 0.1037]	14941 [R_{int} = 0.0793]	28639 [R(int) = 0.0664]	25912 [R_{int} = 0.1306]	20453 [R_{int} = 0.0790]
Data / restraints /parameters	4553 / 0 / 289	7529 / 0 / 320	5015 / 0 / 297	5244 / 10 / 352	14941 / 1 / 876	28639 / 8 / 1640	25912 / 0 / 1617	20453 / 0 / 1302
GOF on F^2	1.048	1.032	0.973	1.060	1.019	1.055	1.021	1.075
R_1 (I>2σ(I))	0.0932	0.0422	0.0326	0.0603	0.0713	0.0570	0.0704	0.0981
wR_2 (all data)	0.2764	0.1131	0.0739	0.1655	0.1863	0.1613	0.1959	0.2963

Theoretical Calculations

Geometry Optimizations and population analyses were performed using Gaussian 16 rev. A.03.[9] Hybrid quantum mechanics/molecular mechanics (QM/MM) optimizations using B3LYP-D3(BJ)/def2-SVP for QM and universal force field (UFF) parameters for MM. All core CAAC-CO_2 and M (M = Li, Na, K) atoms were treated in the QM domain, while Dipp groups and explicit THF molecules were treated in the MM domain UFF. All calculations were inclusive of solvent effects using the polarizable continuum model (IEF-PCM) with Truhlar's SMD model with parameters for THF ($\varepsilon = 7.25$).

All subsequent property and electronic structure calculations employed the QM/MM optimized geometries with a full QM treatment of the entire system. Molecular orbital (MO) and intrinsic bonding orbital (IBO) analysis was performed using single-point B3LYP-D3(BJ)/def2-SVP calculations (inclusive of THF solvation). Hyperfine couplings (HFC) were computed using ORCA 4.2.1 at the B3LYP-D3(BJ)/EPR-II level of theory inclusive of solvent (CPCM(THF)).[10] X-band EPR spectra were simulated with EasySpin 6.0.0-dev.26, using the esfit least-squares fitting function. The Nelder/Mead downhill simplex local optimization algorithm was employed, with an integral target function varying parameters for $\boldsymbol{a}_{\mathbf{iso}}$, and $\boldsymbol{g}$, starting with theoretically computed values, fitting to the experimental spectra.

Spin Populations



2(Li) **3(Na)** **4(K)**

Figure S24. Spin density surface plots of compounds **2-4**. B3LYP-D3(BJ)/def2-SVP//B3LYP-D3(BJ)/def2-SVP/UFF inclusive of THF solvent model.

Table S2. Computed spin population percentages of singly reduced **2-4** for specific atoms and summed for CAAC (except Dipp) and CO2 fragments. The remaining spin population is located on the Dipp (N_{CAAC}) substituents.

	2(Li)		**3(Na)**		**4(K)**	
	Atoms	Fragment	Atoms	Fragment	Atoms	Fragment
CAAC Carbon CAAC Nitrogen	51% 22%	73%	61% 16%	76%	58% 13%	78%
CO2 Carbon CO2 Oxygen	4% 14%	18%	6% 14%	19%	8% 15%	18%
Alkali Metal	0.4%		0.5%		0.6%	
Sum (Heavy Atoms)	97%		99.6%		99.2%	

Simulated EPR Spectra

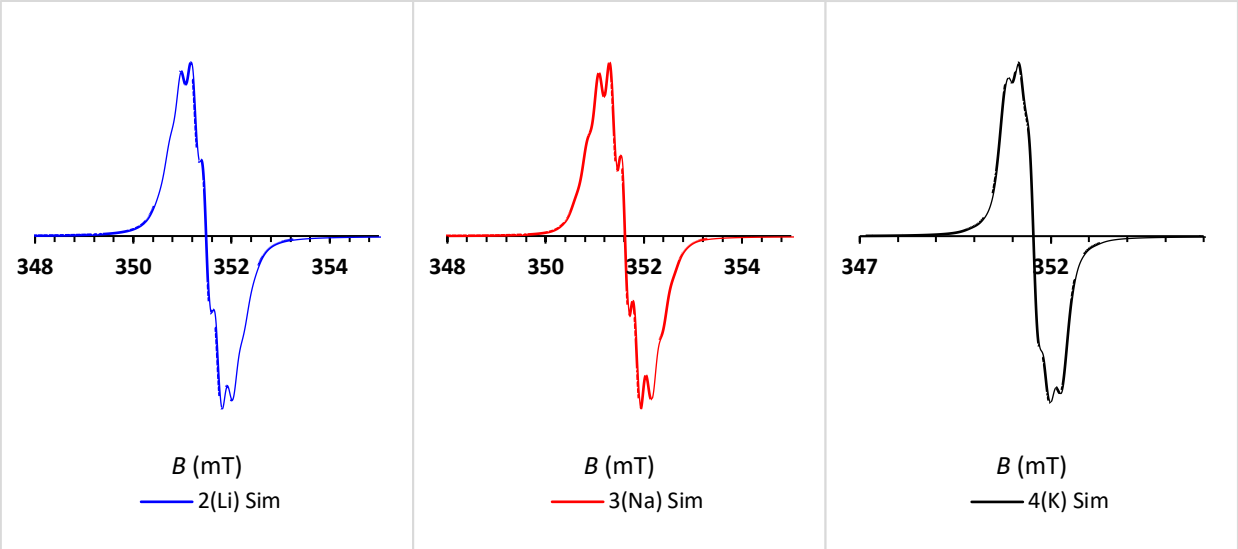


Figure S25. Simulated EPR spectra for **2(Li)**, **3(Na)** and **4(K)**.

Molecular Orbitals

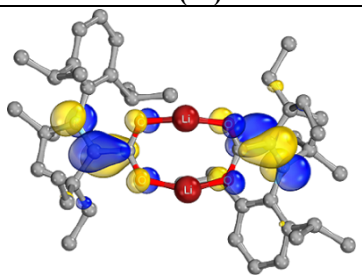
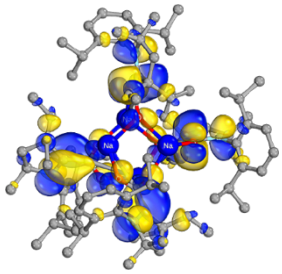
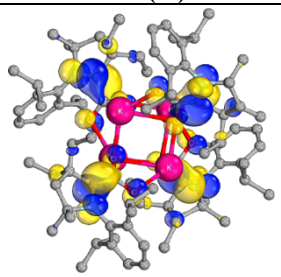
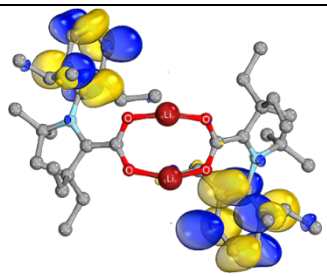
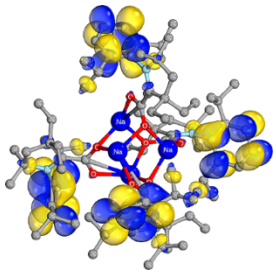
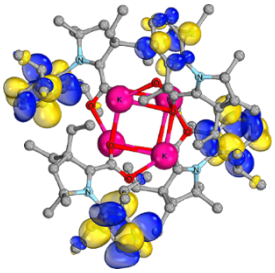
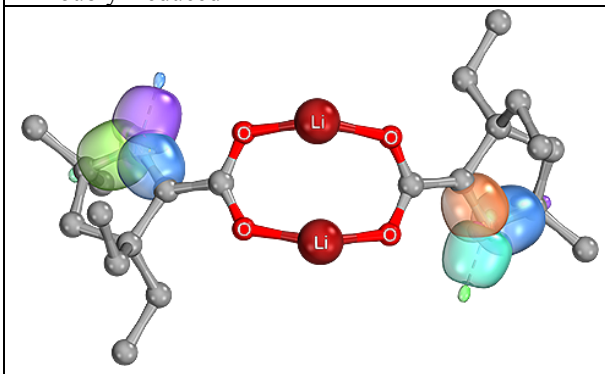
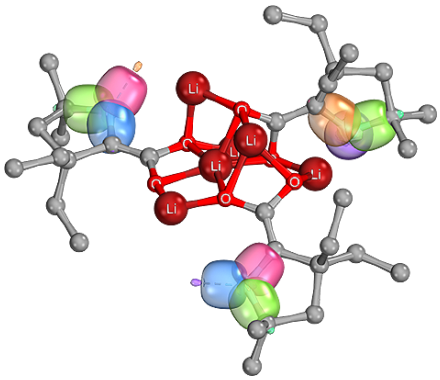
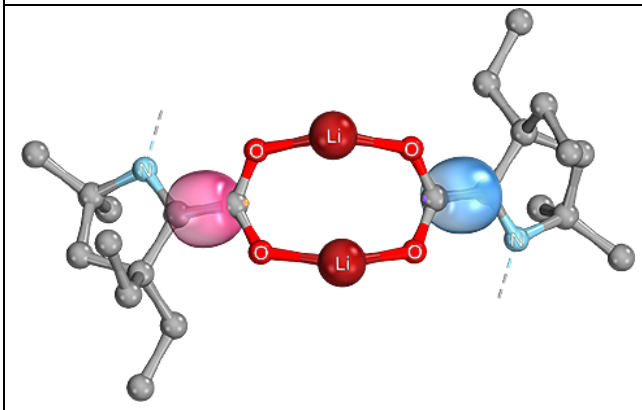
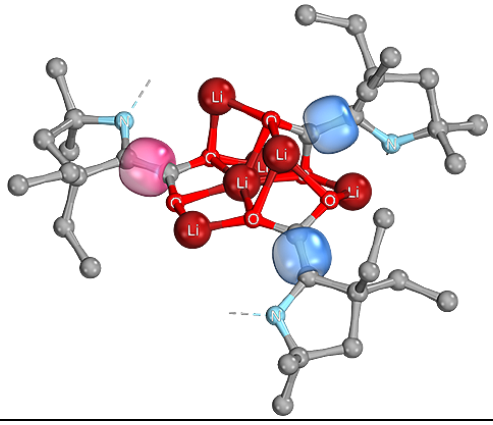
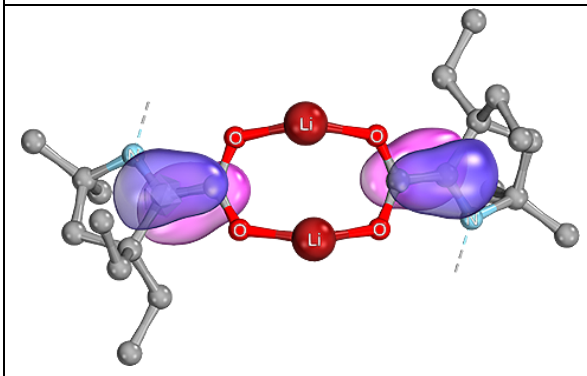
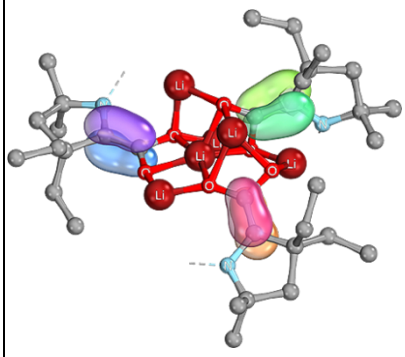
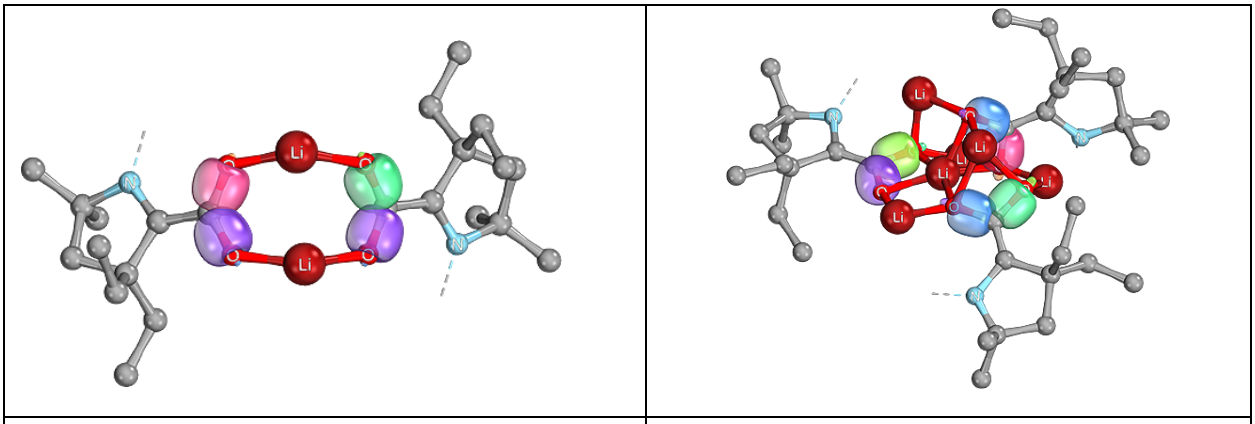
2(Li)	3(Na)	4(K)
		
SOMO	SOMO	SOMO
		
LUMO	LUMO	LUMO

Figure S26. Frontier molecular orbitals of compounds **2-4**. B3LYP-D3(BJ)/def2-SVP//B3LYP-D3(BJ)/def2-SVP/UFF inclusive of THF solvent model.

Intrinsic Bonding Orbitals

2 Doubly-Reduced	**5** Singly-Reduced
	
N_{CAAC} sigma bonds N1- $C_{Carbene}$ σ (N1=1.169; $C_{Carbene}$=0.813) N1- C_{Dipp} σ (N1=1.128; C_{Dipp}=0.855) N1- C_{CAAC} σ (N1=1.143; C_{CAAC}=0.819)	N_{CAAC} sigma bonds N1- $C_{Carbene}$ σ (N1=1.099; $C_{Carbene}$=0.873) N1- C_{Dipp} σ (N1=1.156; C_{Dipp}=0.818) N1- C_{CAAC} σ (N1=1.042; C_{CAAC}=0.930)
	
C-C sigma bond $C_{Carbene}$-C_{CO2} σ ($C_{Carbene}$ =1.020; C_{CO2}=0.962)	C-C sigma bond $C_{Carbene}$-C_{CO2} σ ($C_{Carbene}$ =1.008; C_{CO2}=0.973)
	
C-C pi bond $C_{Carbene}$-C_{CO2} π ($C_{Carbene}$ =1.386; C_{CO2}=0.503)	C-C pi bond $C_{Carbene}$-C_{CO2} π ($C_{Carbene}$ =1.199; C_{CO2}=0.768)



C-O sigma bond C_{CO2}-O_{CO2} π (C_{CO2} =1.223; O_{CO2}=0.771)	C-O sigma bond C_{CO2}-O_{CO2} π (C_{CO2} =1.177; O_{CO2}=0.812)

Figure S27. Carbene and CO_2 IBOs of compounds **2-4**. B3LYP-D3(BJ)/def2-SVP//B3LYP-D3(BJ)/def2-SVP/UFF inclusive of THF solvent model.

Cartesian Coordinates of Optimized Geometries. B3LYP-D3(BJ)/def2-SVP/UFF (IEF-PCM/SMD, THF)

2

Ee = -1511.316585 Hartree

Li	-0.63421341	1.75809390	1.16750805
O	-2.14581241	1.00769990	0.37448805
O	-1.45070941	-1.11189410	0.68811605
O	-1.33308541	3.45869590	2.11891605
O	-0.17792341	0.56505690	2.81015705
N	-4.25824541	0.00019990	-1.44893895
C	-2.28171741	-0.26534510	0.14360405
C	-3.32225341	-0.77507910	-0.68854795
C	-3.55411341	-2.26441910	-0.99305695
C	-4.89326841	-2.26604910	-1.82094495
H	-4.90121141	-2.97139710	-2.66873195
H	-5.73665841	-2.61845810	-1.20317795
C	-5.14727841	-0.79820910	-2.30444295
C	-6.63751841	-0.44064010	-2.13489895
H	-6.98211541	-0.64734110	-1.10331695
H	-7.26597541	-1.05812310	-2.81265495
H	-6.81624241	0.62873090	-2.37490495
C	-4.81570541	-0.66235810	-3.80292495
H	-5.06062441	0.36014790	-4.14931195
H	-5.42547741	-1.37119210	-4.40383395
H	-3.75095541	-0.88250510	-4.00848695
C	-2.36894741	-2.80488610	-1.84643595
H	-2.31020841	-2.24234310	-2.80124895
H	-1.41566641	-2.62162210	-1.31293395
C	-2.41749041	-4.30304310	-2.17257095
H	-1.57614841	-4.55282310	-2.85296195
H	-3.36170541	-4.58511510	-2.67810895
H	-2.29601141	-4.91174410	-1.25278895
C	-3.70696941	-3.12558510	0.29492905
H	-4.16158941	-4.10502910	0.02972705
H	-2.71162041	-3.34920010	0.72598705
C	-4.56832041	-2.49729710	1.39905805
H	-4.09081741	-1.58235110	1.80556105
H	-4.67519341	-3.22140310	2.23391405
H	-5.58271341	-2.24720410	1.02905305
C	-4.30473241	1.42445190	-1.38374095
C	-3.48984141	2.22056490	-2.24842295
C	-3.67855041	3.61111890	-2.27038595
H	-3.08658941	4.24901190	-2.91267895
C	-4.65173841	4.23744990	-1.37817995
H	-4.78745741	5.31096390	-1.38864695
C	-5.32625941	3.45543190	-0.45647495
H	-5.97346241	3.95094590	0.25487005
C	-5.15615841	2.05884090	-0.42487295
C	-5.83524841	1.27377490	0.69662705
H	-5.68683141	0.18739890	0.55255705
C	-5.20510641	1.60404090	2.05572705
H	-4.12504941	1.35388590	2.04877905
H	-5.68732541	1.00203190	2.85541805
H	-5.32207441	2.68050190	2.30282305
C	-7.35255741	1.52308790	0.73838105
H	-7.58676341	2.52630290	1.15258005
H	-7.84145941	0.76158590	1.38280205
H	-7.79454741	1.45564190	-0.27652195
C	-2.35852241	1.63321190	-3.09085195
H	-2.33324141	0.53222490	-2.98580095

C	-0.99124641	2.13990290	-2.60859195
H	-0.92362441	3.24483990	-2.68722195
H	-0.18041741	1.70543790	-3.22932795
H	-0.80946641	1.84531290	-1.55718695
C	-2.52448141	1.96183890	-4.58418395
H	-3.55833241	1.77500090	-4.92950495
H	-1.83596141	1.33110990	-5.18621895
H	-2.28670041	3.02723890	-4.78929995
C	-2.34870041	3.96909290	1.25159505
H	-3.14692941	4.46486090	1.84384605
H	-2.75808041	3.09852790	0.72081905
C	-1.61412741	4.97004490	0.36295005
H	-2.28508041	5.70618390	-0.10751295
H	-1.07936541	4.42770990	-0.43020395
C	-0.61499341	5.60186490	1.34625905
H	0.29818159	5.96168090	0.84971905
H	-1.07617541	6.45944290	1.86593505
C	-0.32115641	4.45404390	2.33549905
H	0.64267859	3.96535090	2.13620805
H	-0.35896141	4.79809790	3.38644205
C	-1.33194741	0.30757390	3.62854905
H	-1.85889141	-0.55562310	3.19847005
H	-1.99817841	1.18566690	3.57724005
C	-0.77870841	0.10826290	5.04088605
H	-0.46321541	-0.93836710	5.18965205
H	-1.51364741	0.35704790	5.82284605
C	0.98560959	0.82601390	3.61422205
H	1.50840659	1.68583790	3.17252705
H	1.64985959	-0.05331510	3.56059105
C	0.44841559	1.03343890	5.03146505
H	0.13502359	2.08100790	5.17835405
H	1.19214259	0.78856390	5.80630605
Li	0.27083159	-0.65415210	1.17764905
O	1.76939359	0.07558190	0.34960605
O	1.08924759	2.20014290	0.66588705
O	0.96568759	-2.33332310	2.16939605
N	3.88847959	1.06550490	-1.47435195
C	1.91563959	1.34848790	0.11977905
C	2.96403459	1.85018490	-0.70545895
C	3.21245359	3.33842790	-1.00551995
C	4.55481759	3.32327790	-1.82756095
H	4.58953759	4.04610490	-2.65976795
H	5.40213259	3.63657190	-1.19459595
C	4.77417459	1.85920790	-2.33778995
C	6.26187259	1.47307490	-2.20751995
H	6.63657259	1.66659990	-1.18425395
H	6.88402259	2.08394390	-2.89687195
H	6.41665259	0.40185790	-2.45676895
C	4.40766159	1.75454990	-3.83134595
H	4.63070359	0.73696390	-4.20294795
H	5.01309259	2.46662790	-4.43275495
H	3.34244459	1.99021590	-4.01203395
C	2.03345559	3.89568390	-1.85806395
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H	-4.21964241	-2.09062893	1.34144953
H	-5.13523241	-3.49788293	0.70876153
C	-3.58619441	-4.07853693	2.12164553
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4

Ee = -4927.378673 Hartree

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C	-1.83197337	-1.10916899	2.42384900
C	-2.72596737	-1.60314899	3.50211800
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Ee = -6619.455052 Hartree

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C	-6.23042337	6.00720159	-0.49240188
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H	-6.28212337	2.35870159	1.86909812
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C	-2.80303778	6.47990084	-5.20322968
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C	0.43473696	-2.85341021	-4.50010874
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H	2.47190003	-5.67827812	-0.52874799
C	3.98590003	-4.97337812	-1.65324799
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C	4.34560003	-4.01767812	-2.56514799
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Li	1.95755232	-1.68168141	0.55270380
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C	-5.35167670	-0.78254278	6.05932500
H	-5.99027670	-1.51304278	6.20352500
H	-5.66337670	0.01965722	6.52772500
H	-4.47367670	-1.04384278	6.40622500
Li	0.14475232	4.45981859	-0.37029620
Li	0.09665232	2.29391859	-1.49649620
Li	-1.46104768	3.12391859	1.35930380
Li	2.37385232	1.05341859	-0.24229620
Li	0.20035232	0.40641859	0.82520380
Li	-0.74244768	-0.55288141	2.76610380

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Ee = -3769.849496 Hartree

O	-0.29214100	7.72849300	16.09934700
O	-0.78036100	7.78215800	13.91337200
O	-2.02564800	5.19593300	15.02131700
O	-3.15010400	6.95282400	15.75813800
O	0.61159500	4.53970300	14.28392800
O	-2.89377400	6.61858100	12.34564800
O	1.58884600	6.47895500	14.58915600
O	2.89190600	7.07182200	17.09833000
N	-1.50979000	9.94020200	16.76350400
N	3.82862100	5.84516700	13.00445900
N	-3.74537100	3.42716900	16.77456500
C	-0.79613300	8.42397600	15.05809300
C	-3.00175000	5.62114300	15.84815500
C	-0.29914300	10.03773200	17.53781200
C	-1.61187700	2.26802000	16.58509100
C	0.83059400	10.73325500	17.08844200
C	3.46571800	7.16449700	12.47746000
C	2.01218600	10.67336800	17.81957200
H	2.88424300	11.17786500	17.43891000
C	2.22917600	7.27341800	11.60110500
C	1.71243700	5.25717600	14.04653200
C	-2.86660100	2.60374800	16.04398300
C	-4.96700000	5.35665300	17.47749600
C	-2.56631700	10.95961400	16.93607900
C	5.32095300	8.17430300	13.88044500
H	5.40697900	7.16042600	14.23052700
C	-1.14704800	2.89622400	17.89579800
H	-1.99931600	3.39525100	18.33011700
C	-4.70975000	2.89275900	17.71556800
C	-3.79163700	4.86588700	16.62811700
C	-0.22969300	9.33932600	18.75132200
C	-0.73351000	1.47199200	15.85998700
H	0.23286600	1.23316700	16.27009500
C	4.96065000	5.10272800	12.43497800
C	-1.41804600	9.58226600	15.33910700
C	-1.39899900	8.51960000	19.29148100
H	-2.23455900	8.62593100	18.62674900
C	-0.07231500	3.97591500	17.60679100
H	0.77298000	3.54684000	17.08549800
H	0.26695900	4.41702900	18.53420600
H	-0.48705500	4.75490200	16.97936000
C	0.81889700	11.57518800	15.81648600
H	-0.18997600	11.60283600	15.45115800
C	2.80014100	4.89598100	13.35962800
C	-3.88213800	10.29547200	17.41608100
H	-4.11802600	9.44920000	16.78691900
H	-4.70170100	11.00080300	17.36877300
H	-3.78292500	9.95141800	18.43540100
C	3.08909400	3.51890000	12.75372600
C	5.71254800	5.83348800	11.29755200
H	5.05624300	5.98669900	10.45482400
H	6.55840800	5.23544200	10.98620800
H	6.05551500	6.79993000	11.62673600
C	-3.97037000	6.94507800	11.48249600
H	-4.21657800	8.00452200	11.58318900
H	-4.84433000	6.35950600	11.77800900
C	-3.18540000	2.18037400	14.74355400
C	-2.27851500	1.40771400	14.02338700
H	-2.51968400	1.10577600	13.01814000
C	4.22409100	8.22865900	12.80681300
C	3.51864100	2.45219600	13.81138300
H	3.96667300	1.60905600	13.30419200
H	4.28385800	2.88940100	14.43271200
C	-1.72708300	6.19717800	11.62837100
H	-1.20206400	5.45041900	12.22452300
H	-1.03799200	7.03630300	11.49352500
C	4.31542100	3.80979000	11.85321800
H	3.97767000	4.02200300	10.85167800
H	5.00880200	2.98553700	11.80897300

C	0.94727900	9.33411600	19.48206200
H	0.98784600	8.78718300	20.40675000
C	2.47654300	6.67567300	10.18286500
H	3.00510100	5.74255500	10.29265900
C	2.07814100	9.98271200	19.01521000
H	3.00048800	9.94299300	19.57084600
C	-6.25147100	5.57233600	16.61552800
H	-6.33700600	4.74041600	15.93337900
H	-7.12517000	5.55506300	17.25334500
C	-2.75552800	11.56271700	15.51696300
H	-2.10935000	12.42044100	15.40884700
H	-3.76930400	11.89499100	15.36547300
C	-0.59311400	1.84285500	18.88970500
H	-1.31688400	1.05902000	19.07197400
H	-0.34986500	2.31791000	19.83215700
H	0.30950100	1.39402700	18.49556500
C	-5.19372100	4.16726100	18.45425600
H	-6.22014200	4.08060300	18.77425200
H	-4.57755100	4.31380900	19.32854100
C	-1.02238100	7.02147800	19.35284800
H	-0.75409800	6.67232800	18.36261500
H	-1.85315200	6.43165900	19.71654800
H	-0.17964900	6.87100200	20.01316100
C	-2.17182100	12.06133700	17.94961000
H	-2.01350500	11.63848100	18.93282200
H	-2.96726700	12.79296100	18.00872300
H	-1.26316200	12.55720500	17.63633900
C	1.89547100	3.01228800	11.90507000
H	1.03297500	2.90656100	12.54750000
H	1.66157800	3.79097000	11.18909000
C	2.37004600	1.95396100	14.71190900
H	1.69147300	1.33241900	14.14892100
H	1.80547800	2.80146100	15.07769400
H	2.74819100	1.37933400	15.54767200
C	1.77600200	8.74054200	11.59923100
H	0.92536500	8.95321900	10.98809100
C	-2.32919900	10.46795800	14.49602500
C	-3.55137500	9.63994500	14.00580000
H	-4.00650700	9.13936300	14.84388600
H	-3.16597400	8.86727600	13.36309800
C	6.00589000	4.74151100	13.54373900
H	6.64371200	5.59131900	13.73975900
H	6.62679100	3.91072500	13.23719900
H	5.49679500	4.48269500	14.45977800
C	-6.23231700	6.88098300	15.79122800
H	-6.36864900	7.74260800	16.42996300
H	-7.02282200	6.87759300	15.05155400
H	-5.27027600	6.98316700	15.29765800
C	3.96002400	9.55839200	12.25264500
H	4.66042500	10.34265600	12.41410500
C	-4.47179100	2.63955700	14.06278500
H	-5.03032000	3.20885500	14.79045900
C	3.90389800	6.31804900	16.42446800
H	4.89093300	6.69673000	16.70204400
H	3.74965700	6.40864400	15.34750700
C	2.74346600	9.76561600	11.69266000
H	2.48527900	10.76286300	11.36420500
C	-1.06331300	1.03686900	14.58219200
H	-0.36431100	0.44114800	14.01548800
C	1.26534300	13.03270700	16.11619100
H	0.67076000	13.47371500	16.90617500
H	1.15716800	13.63379800	15.22144600
H	2.30486100	13.05718300	16.41438200
C	4.90477700	9.07514300	15.07734600
H	4.87778700	10.10660400	14.75551300
H	5.59289500	8.98443400	15.90800500
H	3.91105100	8.80582700	15.41075000
C	1.72307300	10.95658100	14.71954200
H	2.73906000	10.85667700	15.07361200
H	1.73001900	11.58162800	13.83534200
H	1.36850000	9.97521800	14.40695600
C	-4.64412900	6.63139600	18.29498800
H	-4.46515700	7.44166700	17.60971700
H	-3.72387700	6.46000600	18.83268300
C	-4.09817100	1.87518500	18.72365300
H	-3.61877700	1.06372100	18.19187100
H	-4.88441300	1.46531800	19.34331500
H	-3.36958600	2.34804100	19.36363900
C	-5.89572400	2.14530500	17.02671800
H	-6.42046300	2.78575700	16.33567800
H	-6.59514200	1.80047700	17.77628800
H	-5.51887800	1.28800500	16.48687500
C	-1.67449200	11.17955100	13.27145500
H	-2.31277300	12.00617600	12.98872400
H	-0.72777200	11.59826200	13.57766300
C	3.32237900	7.60400400	9.25333700
H	2.75482900	8.49896700	9.04247600
H	3.58669400	7.13094000	8.31577700
H	4.22354200	7.90852300	9.76757500
C	1.13275600	6.35609100	9.47695800
H	0.60747800	5.61065900	10.05495700
H	1.26320200	5.99416400	8.46413500
H	0.52603200	7.25002000	9.44918400
C	6.71840400	8.65741800	13.39517300
H	7.11816900	8.01769000	12.62262900
H	7.42207100	8.67517700	14.21776200
H	6.63648300	9.65778800	12.99335200
C	-1.86005800	9.02564200	20.68324300
H	-1.06478300	8.91542400	21.40890100
H	-2.71581300	8.45214600	21.01964000
H	-2.13940300	10.07094800	20.63675000
C	-5.75947200	7.03384800	19.29105200
H	-6.68153200	7.24344900	18.76524500
H	-5.47168900	7.92457600	19.83676000
H	-5.94745500	6.24277600	20.00495400
C	3.26021100	5.09806800	18.41014800

H	4.12172100	5.08019800	19.06506000
H	2.55360100	4.35462700	18.75249600
C	3.68263900	4.87462800	16.93520900
H	2.87975600	4.42441200	16.36018300
H	4.56782200	4.26042500	16.83778700
C	2.17207300	1.67789300	11.16508700
H	3.05430200	1.76627800	10.54442100
H	1.33622500	1.41009400	10.53065600
H	2.33387200	0.87289700	11.86905800
C	-3.49849700	6.59073400	10.03600000
H	-4.28344700	6.11842200	9.46059000
H	-3.17954000	7.48761600	9.51835200
C	-4.13942800	3.57546200	12.87297200
H	-3.57381000	4.43073600	13.22719000
H	-5.05071700	3.92435300	12.40431200
H	-3.54732000	3.05230900	12.13368400
C	-4.62752700	10.44340700	13.23559000
H	-4.21077600	10.89364600	12.34486100
H	-5.04496200	11.22999700	13.84924000
H	-5.43625900	9.78644400	12.93894200
C	-1.42234400	10.27423600	12.04675500
H	-0.89958300	10.83127000	11.27951800
H	-2.34485200	9.89891600	11.63067200
H	-0.79360500	9.43596600	12.33223700
C	-5.32542300	1.43962000	13.57281400
H	-4.79672600	0.89460600	12.80148200
H	-6.26000000	1.79634300	13.15743100
H	-5.54531700	0.75797500	14.38388100
C	-2.28432500	5.66047400	10.28288000
H	-1.54328600	5.72436800	9.49609200
H	-2.60391000	4.63120800	10.38687600
C	2.62246900	6.52805900	18.38526300
H	1.54341800	6.49793100	18.51638400
H	3.04694300	7.17296500	19.15917500
Li	1.04108100	7.54210600	13.10796800
Li	-2.37893300	6.89441300	14.05003400
Li	-0.23541800	6.16843800	14.89916100
Li	1.55236900	7.52078800	15.94759800
Li	-0.90651300	3.95236500	14.48636400
Li	-2.06619800	8.00048200	16.66073000

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Ee = -8461.081584 Hartree

Na	-0.63349944	0.60588982	-2.23846790
Na	-2.07209944	3.76208982	-3.08086790
Na	-2.06929944	2.28958982	-0.19436790
Na	-1.36095993	5.54779271	0.71728080
Na	0.41490056	2.58638982	1.41743210
Na	1.80630056	0.65318982	-0.41386790
Na	-0.64189944	0.21368982	3.03883210
Na	4.01190056	-1.89801018	0.20543210
Na	1.78240056	-2.23441018	3.89413210
Na	0.61440056	-1.65081018	0.95283210
Na	-1.83129944	-1.79811018	-0.79116790
Na	-3.17629944	-0.10671018	1.22803210
O	-2.96986346	0.16204752	-0.98486926
O	-2.53829944	1.70788982	-2.60186790
O	-1.06148756	4.17046953	-1.06041341
O	0.35100056	2.29318982	-0.89456790
O	-1.32745993	3.80169271	2.05668080
O	-2.10139944	1.62008982	2.09653210
O	1.37000980	0.67782941	1.88551060
O	2.62720056	-1.27191018	1.90453210
O	-0.26629944	-1.97561018	3.18193210
O	-1.72103653	-1.83131835	1.40404345
O	2.55996698	-1.21253100	-1.28989336
O	0.29130056	-1.26961018	-1.35216790
N	-4.88732804	0.89378713	-4.16676971
N	0.60374286	5.49777029	-2.91263437
N	-3.00072154	4.60872348	4.26677490
N	4.29240462	-0.43941745	4.02667072
N	-2.09128373	-3.64815716	4.72337008
N	2.81088915	-2.88592927	-3.63315227
C	-3.37776346	0.73284752	-2.15496926
C	-4.55864761	0.40672860	-2.80842776
C	-5.61094761	-0.65957140	-2.41772776
C	-6.46294761	-0.76097140	-3.70182776
H	-6.65734761	-1.70997140	-3.90592776
H	-7.32294761	-0.28627140	-3.57642776
C	-5.67464761	-0.12567140	-4.85522776
C	-4.79934761	-1.20497140	-5.52992776
H	-4.39474761	-0.83597140	-6.34272776
H	-5.35514761	-1.97757140	-5.76352776
H	-4.09284761	-1.48577140	-4.91172776
C	-6.58914761	0.49172860	-5.90042776
H	-7.18754761	1.13782860	-5.47052776
H	-7.12094761	-0.21267140	-6.32642776
H	-6.04844761	0.94802860	-6.57842776
C	-4.97884761	-1.98277140	-2.03702776
H	-4.41214761	-1.83477140	-1.23852776
H	-4.38044761	-2.26187140	-2.77472776
C	-5.94384761	-3.15217140	-1.73312776
H	-6.53544761	-3.29627140	-2.49942776
H	-6.48094761	-2.93467140	-0.94142776
H	-5.42624761	-3.96667140	-1.56072776
C	-6.57974761	-0.14207140	-1.29812776
H	-7.01204761	0.68642860	-1.62622776
H	-7.29454761	-0.81647140	-1.17602776
C	-5.97994761	0.14912860	0.04927224
H	-5.27634761	0.82392860	-0.04532776
H	-5.59754761	-0.67287140	0.42077224
H	-6.67704761	0.48592860	0.65097224
C	-4.68462804	2.21938713	-4.64426971
C	-3.62992804	2.48198713	-5.54376971
C	-3.42482804	3.79538713	-6.00216971
H	-2.70912804	3.97418713	-6.60096971

C	-4.24702804	4.83338713	-5.59676971
H	-4.08382804	5.72018713	-5.89566971
C	-5.30122804	4.56598713	-4.75796971
H	-5.87642804	5.27538713	-4.49826971
C	-5.54912804	3.27248713	-4.27436971
C	-6.74912804	3.04228713	-3.39936971
H	-6.89442804	2.05438713	-3.34546971
C	-8.03792804	3.66598713	-3.96156971
H	-7.95112804	4.64218713	-3.97086971
H	-8.79732804	3.41108713	-3.39716971
H	-8.18612804	3.34258713	-4.87456971
C	-6.47932804	3.54528713	-1.97406971
H	-5.68972804	3.09218713	-1.61166971
H	-7.25552804	3.35188713	-1.40726971
H	-6.32182804	4.51208713	-1.99296971
C	-2.72582804	1.38538713	-6.04116971
H	-2.97262804	0.54228713	-5.56306971
C	-1.25402804	1.68608713	-5.74186971
H	-0.97762804	2.48728713	-6.23416971
H	-0.70222804	0.92548713	-6.02006971
H	-1.14022804	1.83798713	-4.78056971
C	-2.93192804	1.15438713	-7.54886971
H	-3.87192804	0.93678713	-7.72076971
H	-2.36522804	0.41208713	-7.84576971
H	-2.68972804	1.96708713	-8.03986971
C	0.08230450	3.54270389	-1.45723087
C	0.92715288	4.13345796	-2.38982406
C	2.18005288	3.56035796	-3.07922406
C	2.60275288	4.75745796	-3.96462406
H	3.34925288	5.24765796	-3.53652406
H	2.91005288	4.43275796	-4.84822406
C	1.39325288	5.68835796	-4.13812406
C	1.83775288	7.14415796	-4.30112406
H	1.04955288	7.71825796	-4.39282406
H	2.39775288	7.22715796	-5.10152406
H	2.35255288	7.41885796	-3.51332406
C	0.54235288	5.29395796	-5.34632406
H	0.14955288	4.40895796	-5.19462406
H	1.10445288	5.26895796	-6.14852406
H	-0.17394712	5.95195796	-5.46992406
C	1.81275288	2.34305796	-3.96112406
H	1.36825288	1.66925796	-3.38852406
H	1.15335288	2.63845796	-4.63712406
C	2.96885288	1.66105796	-4.68922406
H	3.41615288	2.30955796	-5.27222406
H	2.62285288	0.92035796	-5.22972406
H	3.60985288	1.31515796	-4.03342406
C	3.29165288	3.09305796	-2.08232406
H	3.07075288	3.44535796	-1.18362406
H	3.26425288	2.10495796	-2.02782406
C	4.72475288	3.51845796	-2.42912406
H	4.90185288	3.33065796	-3.37452406
H	5.35765288	3.01805796	-1.87262406
H	4.83055288	4.47825796	-2.26132406
C	0.38924286	6.57827029	-1.99313437
C	1.28184286	6.90187029	-0.95853437
C	0.94984286	7.95797029	-0.09533437
H	1.53164286	8.15727029	0.62846563
C	-0.19695714	8.72027029	-0.25883437
H	-0.38485714	9.44367029	0.32736563
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