Electronic Supplementary Information for

Radical anions of 1,1-azoliumdithiocarboxylates

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Author contributions

M.S.L. and U.R. conceived of the project; M.S.L. did most of the experimental, K.O. added CV and SC-XRD analyses I. K. EPR spectroscopy, U.R. quantum-chemical calculations.; M.S.L., U.R. and H.B. wrote the manuscript.

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1 Additional Figures, Tables and Discussions

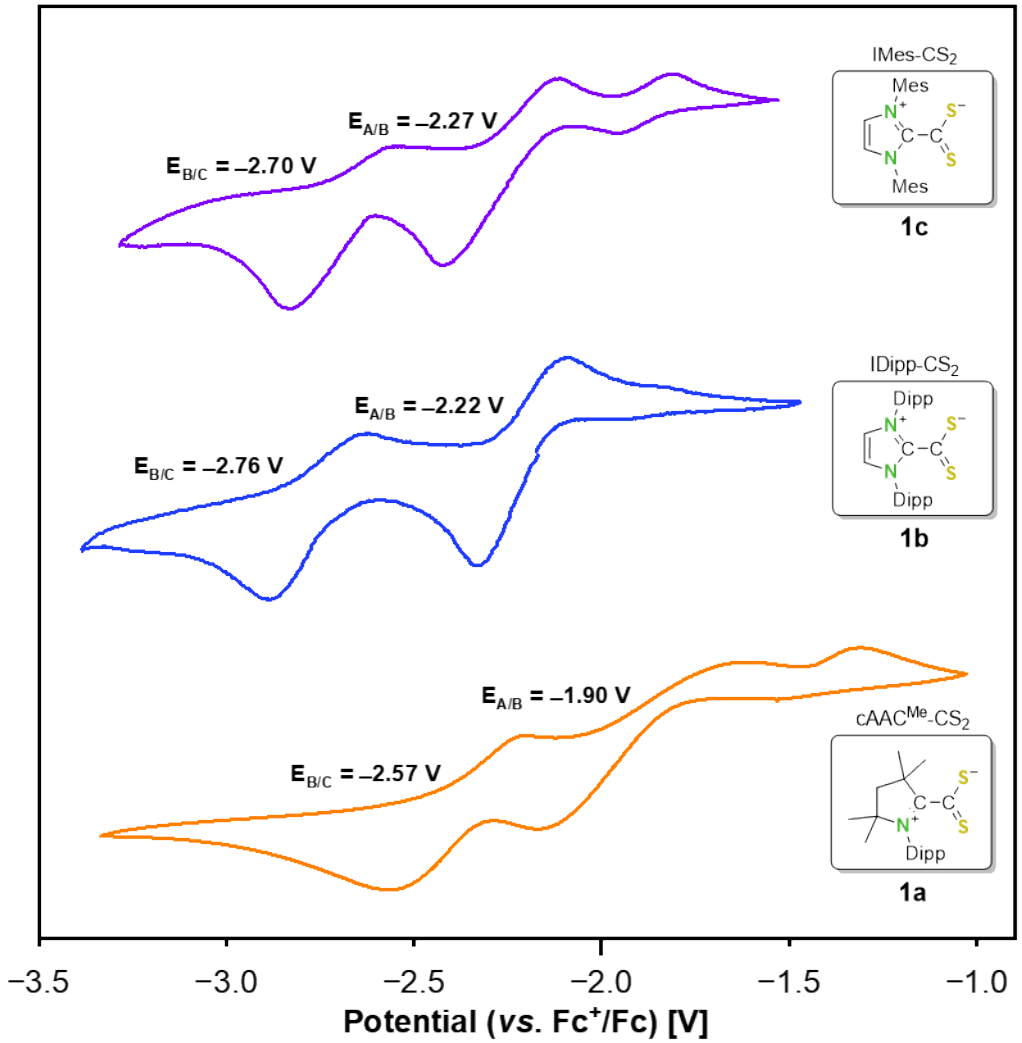


Figure S1. Cyclic voltammograms of the **A**/**B**, **B**/**C** redox-couples (see Scheme 3 of the main text) of the carbene-CS_2 compounds **1a**–**c** in THF (concentrations *ca.* 1 mM) and [TBA][PF_6] (TBA = tetra(*n*-butyl)ammonium; 0.1 M) as electrolyte. Potentials were internally referenced relative to the ferrocenium/ferrocene (Fc^+/Fc) redox-couple with negative sweep directions. For clarity, due to varying resolution of the redox-events at different scan velocities (*v*), the curves containing the best separation of the occurring redox-events are shown in the region between –0.8 V and –3.5 V at different values of *v* (cAAC^{Me}-CS_2 (**1a**): 25 mV/s; IDipp-CS_2 (**1b**): 50 mV/s; IMes-CS_2 (**1c**): 10 mV/s).

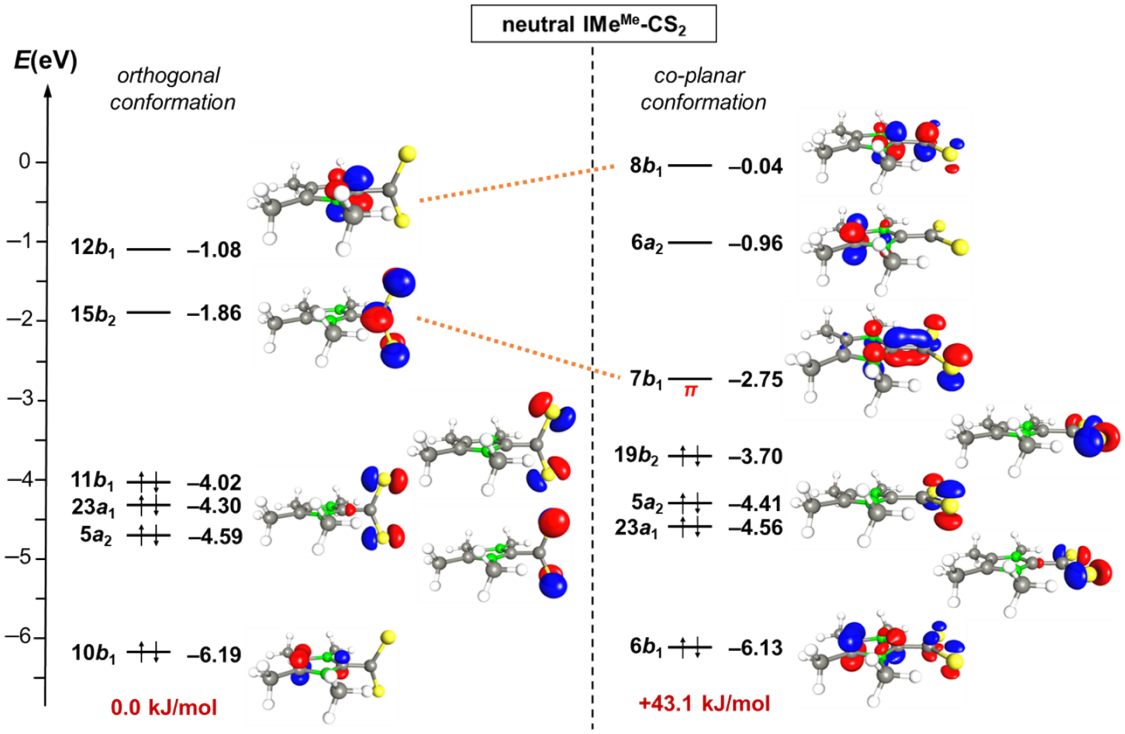
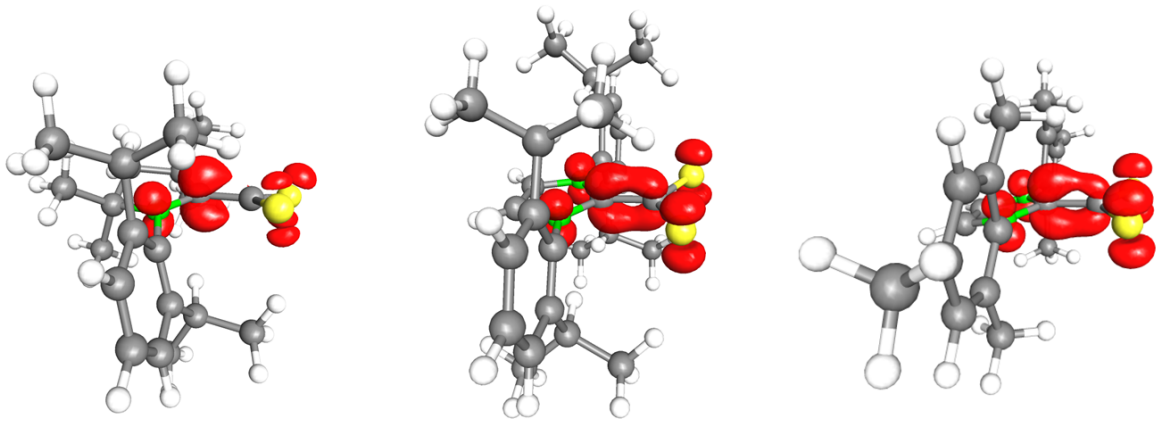


Figure S2. Quantum-chemical DFT calculations (B3LYP/def2-TZVP) of IMe^{Me}-CS_2 in an ideal orthogonal- (left) and a co-planar (right) conformation of the CS_2-moiety relative to the plane of the carbene ring (C_{2V} restricted symmetry).

To gain insight into a theoretical description of the bonding situation present in radical mono-anions of the type [carbene-CS_2]$^{\bullet-}$, a row of DFT calculations were performed at the B3LYP/def2-TZVP level of theory (for details see section 9). To evaluate the important frontier molecular orbitals (FMOs) of NHC-substituted dithiocarboxylates on an easy-to-analyze system and to save computational effort these calculations have been performed on the model system IMe^{Me}-CS_2 (Figure S2). The neutral molecule IMe^{Me}-CS_2 was optimized in symmetry-restricted orthogonal and co-planar conformations.

The orthogonal alignment of the CS_2 moiety relative to the plane of the carbene ring is favored by 43.1 kJ/mol for neutral IMe^{Me}-CS_2 with respect to a co-planar alignment. Rotation of the CS_2 moiety of the orthogonal structure along the central C–C axis by 90 ° into the carbene plane does essentially not affect the occupied orbitals too much but switches on π-interaction between the carbene and the CS_2-moiety. Upon planarization the MOs 15b_2 (CS_2-centered) and 12b_1 (carbene-centered) mix into the π-bonding orbital 7b_1 and the π^*-anti-bonding orbital 8b_1, highlighted in orange dashes in Figure S2. These orbitals are unoccupied for the neutral dithiocarboxylates, and the π-bonding orbital 7b_1 is the LUMO of neutral, co-planar IMe^{Me}-CS_2. This orbital becomes occupied upon reduction of the neutral carbene-CS_2 adducts to yield the mono- and di-anionic forms **B** and **C**, which is in line with the observed changes in the C–C distances for **2a**–**c** and **3** as presented above.

Calculations on the orthogonal and in-plane structure of the anionic $[IMe^{Me}\text{-}CS_2]^{\bullet-}$ radical show that the orthogonal conformer, in which the additional electron is either located at the carbene (SOMO: $15b_2$) or at the CS_2 group (SOMO: $12b_1$) are 133.3 kJ/mol and 75.2 kJ/mol, respectively, higher in energy compared to the in-plane *p*-radical (SOMO: $7b_1$), in which the additional electron is delocalized. The calculated energy minimum structure of the non-constrained radical mono-anion $[IMe^{Me}\text{-}CS_2]^{\bullet-}$ confirms a slightly twisted conformation with a ∡NCCS dihedral angle of 29.7 °, which is favored by 10.3 kJ/mol over the symmetry-restricted co-planar form.



$[cAAC^{Me}\text{-}CS_2]^{\bullet-}$ **$[IDipp\text{-}CS_2]^{\bullet-}$** **$[IMes\text{-}CS_2]^{\bullet-}$**

Figure S3. DFT (B3LYP/def2-TZVP) spin-density of the radical anions $[cAAC^{Me}\text{-}CS_2]^{\bullet-}$, $[IDipp\text{-}CS_2]^{\bullet-}$ and $[IMes\text{-}CS_2]^{\bullet-}$ obtained from quantum-chemical calculations.

Table S1. Selected structural parameters of the compounds cAAC^{Me}-CS_2 (**1a**), [K(THF)(18-crown-6)(cAAC^{Me}-CS_2)] (**2a·THF**), [K(18-crown-6)(IDipp-CS_2)] (**2b**), [Mg(^{Dipp}NacNac)(cAAC^{Me}-CS_2)] (**3**) and comparable literature-known systems. Bond lengths in Å and angles in °.

	d(C–S)	*d*(C–C)[a]	*d*(C–N)[b]	*d*(S–K/Mg)	∢SCS	*Twist-angle* (∢NCCS)
cAAC^{Me}-CS_2 (1a)	1.653(3), 1.681(3)	1.485(3)	1.307(3)	–––	131.0(1)	83.7(3)
IDipp-CS_2 (1b)[1]	1.665(2), 1.651(2)	1.495(3)	1.326(2), 1.326(2)	–––	131.5(1)	92.0(2), 88.0(2)
IMes-CS_2 (1c)[1]	1.667(3), 1.669(3)	1.483(8), 1.489(7)	1.336(5), 1.342(5)	–––	129.1(4)	65.3(2), 62.0(4)
[K(THF)(18-crown-6) (cAAC^{Me}-CS_2)] (2a·THF)	1.728(2), 1.723(3)	1.410(3)	1.393(3)	3.116(1), 3.351(1)	117.9(1)	10.9(3)
[K(18-crown-6)(IDipp-CS_2)] (2b)[c]	1.709(1), 1.737(9)	1.415(1)	1.375(1), 1.386(1)	3.221(1), 3.247(1)	122.5(1)	29.1(1), 31.3(1)
[K(18-crown-6)(IMes-CS_2)] (2c)	1.734(3), 1.733(3)	1.407(5)	1.388(4), 1.387(4)	3.216(1), 3.212(8)	124.0(2)	31.2(4), 31.8(4)
[Mg(^{Dipp}NacNac)(cAAC^{Me}-CS_2] (3)	1.736(2), 1.727(2)	1.420(2)	1.358(2)	2.443(1), 2.430(1)	115.8(1)	0.0(2)
[I*i*Pr^{Me}-CS_2]$^{2-}$ [2]	1.803(8), 1.764(11)	1.375(13)	1.455(10), 1.454(15)	3.156^{avg}	117.6(5)	4.8(14), 8.4(14)

[a] Regarding the bond between the CS_2 group and the carbenic carbon atom. [b] Regarding the bond to the carbenic carbon atom. [c] Structure obtained from a co-crystal of **2b** with the neutral adduct **1b** (87:13).

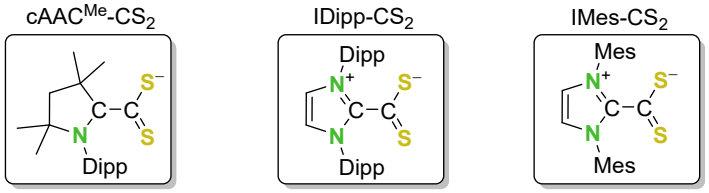
2 Experimental Section

2.1 General Information

All reactions and subsequent manipulations involving organometallic reagents were performed under argon atmosphere by using standard Schlenk techniques or in a Glovebox (Innovative Technology Inc. and MBraun Uni Lab) as reported previously.[3] All reactions were carried out in oven-dried glassware. Benzene, MeCN, THF, toluene, dichloromethane and *n*-hexane were obtained from a solvent purification station (Innovative Technology) by previous purification through alumina columns and then freshly distilled (THF, *n*-hexane, benzene) from sodium as a drying agent with benzophenone as an indicator. The deuterated solvents were purchased from Sigma-Aldrich and dried thoroughly over molecular sieves. The NHCs (= IMes, IDipp)[4] and cAAC^{Me}[5] as well as the reductants [{Mg(^{Dipp}NacNac)}$_2$][6] and KC_8[7] were prepared according to published procedures. The 1,1-azoliumdithiocarboxylates were prepared according to adapted literature procedures.[1] 18-crown-6 was commercially obtained from Sigma-Aldrich and recrystallized from dry acetonitrile prior to use. Elemental analyses were performed in the microanalytical laboratory of the University of Würzburg with an Elementar Vario Micro Cube. Determinations of the magnetic moments were performed according to *Evans*' method using approximately 10–20 mg of the isolated or *in-situ* generated products. For this, frequency shifts were measured using ^{1}H NMR spectroscopy by detection of the shift of the residual proton signals of the deuterated solvents in solution containing the paramagnetic samples relative to the respective shift of an added sealed glass capillary containing the respective neat deuterated solvent.[8]

2.2 Experimental details

General synthesis for 1,1-azoliumdithiocarboxylates:[1]



CS_2 (2.0 eq.) was added to a solution of the carbene (1.0 eq., batch sizes *ca*. 0.5 g – 4.0 g) in THF (20 mL). After stirring at room temperature for 1 h, all volatiles were evaporated *in vacuo.* The residue was suspended in *n*-hexane. After filtration the residue was washed with *n*-hexane (3 x 10 mL) and dried *in vacuo* to afford the 1,1-azoliumdithiocarboxylates (**1a**–**c**) as red to orange solids in yields of 72–94%. The spectroscopical data obtained for **1b** and **1c** match the values reported in literature.

Literature known compounds:

IDipp-CS_2 (1b)[1]

IDipp-CS_2 (**1b**) was synthesized according to the general route using 1.0 eq of IDipp (2.00 g, 5.15 mmol) and 2.0 eq of CS_2 (783.7 mg, 621.9 µL, 10.3 mmol). **Yield**: 91% (2.19 g, 4.70 mmol) of a red solid. **^{1}H NMR** (400.1 MHz, $CDCl_3$): δ = 7.43 (m, 2H, *para*-C*H*), 7.23 (m, 4H, *meta*-C*H*), 7.01 (s, 2H, C$H_{backbone}$), 3.00 (sept, 4H, $^3J_{H\text{-}H}$ = 8.0 Hz, C$H_{methine}$), 1.33 (d, 12H, $^3J_{H\text{-}H}$ = 8.0 Hz, C$H_{3\ methine}$), 1.15 (d, 12H, $^3J_{H\text{-}H}$ = 8.0 Hz, C$_{methine}$-CH_3) ppm. **^{13}C{^{1}H} NMR** (100.6 MHz, $CDCl_3$): δ = 219.7 (CS_2), 149.1 (N*C*N), 146.5 (*ortho*-*C*H$_{aryl}$), 131.4 (*para*-*C*H$_{aryl}$),130.8 (*ipso*-*C*$_{aryl}$), 124.6 (*meta*-*C*$_{aryl}$), 120.6 (*C*H$_{backbone}$), 29.5 (*C*H$_{methine}$), 26.0 (*C*H$_{3,\ Dipp}$), 22.8 (*C*H$_{3,\ Dipp}$) ppm. **CV** (*v* = 50 mV/s, THF): *U* = –2.76 (q. rev., 1e$^-$), –2.22 (q. rev., 1e$^-$) V.

IMes-CS_2 (1c)[1]

IMes-CS_2 (**1c**) was synthesized according to the general route using 1.0 eq of IMes (622.8 mg, 2.05 mmol) and 2.0 eq of CS_2 (311.5 mg, 247.2 µL, 4.09 mmol). **Yield**: 81% (633.0 mg, 1.66 mmol) of a red solid. **^{1}H NMR** (400.1 MHz, d_6-DMSO): δ = 7.84 (s, 2H, C$H_{backbone}$), 7.03 (s, 4H, *meta*-C*H*), 2.28 (s, 6H, *para*-CH_3), 2.23 (s, 12H, *ortho*-CH_3) ppm. **^{13}C{^{1}H} NMR** (100.6 MHz, d_6-DMSO): δ = 221.6 (CS_2), 146.7 (NCN), 139.8 (*C*$_{aryl}$), 135.3 (*C*$_{aryl}$),131.1 (*C*$_{aryl}$), 129.0 (*meta*-*C*H$_{aryl}$), 121.2 (*C*H$_{backbone}$), 20.5 (*para*-*C*H$_3$), 18.1 (*ortho*-*C*H$_3$) ppm. **CV** (*v* = 10 mV/s, THF): *U* = –2.70 (q. rev., 1e$^-$), –2.27 (q. rev., 1e$^-$) V.

Novel Compounds:

Synthesis of cAAC^{Me}-CS$_2$ (1a)

cAAC^{Me}-CS$_2$ (**1a**) was synthesized according to the general route using using 1.0 eq of cAAC^{Me} (3.90 g, 13.7 mmol) in THF (25 mL) and 2.0 eq. of CS$_2$ (2.08 g, 1.65 mL, 27.3 mmol). Single crystals of the product suitable for X-ray diffraction were grown by evaporation of a saturated solution of the product in dichloromethane. **Yield**: 79% (3.91 g, 10.81 mmol) of a red solid. **Elemental analysis**: $C_{21}H_{31}NS_2$ [361.61 g/mol] found (calc.): C 69.69 (69.75), H 8.80 (8.64), N 3.89 (3.87), S 17.89 (17.73)%. **^{1}H NMR** (C_6D_6, 400.1 MHz): δ = 7.04 – 7.00 (m, 1H, CH_{aryl}), 6.94 – 6.92 (m, 2H, CH_{aryl}), 3.01 (sept, $^3J_{H\text{-}H}$ = 6.6 Hz, 2H, C$H_{methine}$), 1.55 (s, 2H, CH_2), 1.54 (s, 6H, N-C(CH_3)$_2$), 1.45 (d, $^3J_{H\text{-}H}$ = 6.6 Hz, 6H, C$_{methine}$-CH_3), 1.09 (d, $^3J_{H\text{-}H}$ = 6.6 Hz, 6H, C$_{methine}$-CH_3), 0.93 (s, 6H, C-C(CH_3)$_2$) ppm. **^{13}C{^{1}H} NMR** (C_6D_6, 100.6 MHz): δ = 226.6 (CS_2), 187.5 (C*C*N), 147.1 (C_{aryl}), 138.3 (C_{aryl}), 130.5 (C_{aryl}), 130.0 (C_{aryl}), 126.3 (C_{aryl}), 125.0 (C_{aryl}), 75.6 (N-*C*(CH$_3$)$_2$), 50.9 (N-C(*C*H$_3$)$_2$), 47.8 (*C*-(CH$_3$)$_2$), 33.0 (N-C(*C*H$_3$)$_2$), 29.8 ($C_{methine}$), 28.5 (CH_2), 28.4 (C$_{methine}$-*C*H$_3$), 25.7 (C$_{methine}$-*C*H$_3$) ppm. **UV/VIS/NIR** (C_6H_6, 298 K): λ_{abs} = 306, 381 nm. **IR** (ATR [cm^{-1}]): ν = 2963 (m), 2923 (w), 2865 (w), 1584 (w), 1527 (s), 1472 (m), 1457 (m), 1388 (m), 1374 (m), 1366 (m), 1345 (m), 1326 (m), 1281 (w), 1210 (w), 1193 (w), 1178 (m), 1148 (m), 1124 (m), 1094 (m), 1075 (m), 1035 (vs), 1019 (s), 979 (m), 960 (m), 948 (m), 809 (m), 772 (s), 731 (m), 715 (w), 698 (s), 602 (m), 564 (m), 542 (m), 485 (m), 436 (m). **CV** (v = 25 mV/s, THF): –2.30 (q. rev., 1e$^-$), –1.90 (q. rev., 1e$^-$) V.

Synthesis of [K(18-crown-6)(cAAC^{Me}-CS$_2$)] (2a)

KC_8 (18.7 mg, 138.3 μmol, 1.0 eq.) and 18-crown-6 (43.9 mg, 165.9 μmol, 1.2 eq.) was added to a solution of cAAC^{Me}-CS$_2$ (50.0 mg, 138.3 μmol, 1.0 eq.) in THF (5 mL) and ultrasonicated for two hours, then stirred at room temperature for another 18 hours. The mixture was filtered through a pad of celite and the remaining solid and the filter pad were extracted with THF (10 mL). *n*-Hexane (10 mL) was added to the filtrate and the clear solution was placed in a freezer at –30 °C. After two days the precipitate was collected by filtration and washed with *n*-hexane (15 mL) yielding [K(18-crown-6)(cAAC^{Me}-CS$_2$)] (**2a**) as green needles. Additional material of **2a** may be obtained by further crystallization from the mother liquor. Single crystals of **2a** suitable for X-ray diffraction were obtained by diffusion of *n*-hexane into a saturated solution of the product in THF at –30 °C. **Yield**: 33% (30.0 mg, 45.1 μmol). **Elemental analysis**: $C_{33}H_{55}KNO_6S_2$ [665.02 g/mol] found (calc.): C 59.76 (59.60), H 8.24 (8.34), N 2.17 (2.11), S 9.25 (9.64)%. **Magnetic moment** (*Evans*' method, d_8-THF): μ_{eff} = 1.36 μ_B. **EPR** (THF, 298 K): g_{iso} = 2.013, a(^{14}N, 1N) = 11.2 MHz. **UV/VIS/NIR** (THF, 298 K): λ_{abs} = 791 nm. **IR** (ATR [cm^{-1}]): ν = 2893 (m), 2863 (m), 1603 (m), 1469 (w), 1453 (w), 1435

(w), 1371 (w), 1350 (m), 1325 (w), 1316 (w), 1283 (w), 1249 (w), 1200 (w), 1104 (vs), 1008 (w), 961 (s), 838 (m), 810 (m), 798 (m), 691 (w), 636 (vw), 607 (vw), 570 (vw), 530 (vw), 479 (vw).

Synthesis of [K(18-crown-6)(IDipp-CS_2)] (2b)

KC_8 (23.3 mg, 172.1 *µ*mol, 1.0 eq.) and 18-crown-6 (54.6 mg, 206.6 *µ*mol, 1.2 eq.) was added to a solution of IDipp-CS_2 (80.0 mg, 172.1 *µ*mol, 1.0 eq.) in THF (5 mL) and ultrasonicated for two hours, then stirred at room temperature for another 18 hours. The mixture was filtered through a glass wool filter, *n*-hexane (40 mL) was added to the filtrate and the clear solution was placed in a freezer at –30 °C. After two days the precipitate formed was collected by filtration and washed with *n*-hexane (15 mL) yielding [K(18-crown-6)(IDipp-CS_2)] (**2b**) as a dark-blue solid. Additional material of **2b** may be obtained by further precipitation from the mother liquor. Single crystals of **2b** suitable for X-ray diffraction were obtained by diffusion of *n*-hexane into a saturated solution of the product in THF at –30 °C. **Yield**: 28% (37.5 mg, 48.8 *µ*mol). **Elemental analysis**: $C_{40}H_{60}KN_2O_6S_2$ [768.15 g/mol] found (calc.): C 62.35 (62.55), H 7.96 (7.96), N 3.69 (3.65), S 8.73 (8.35)%. **Magnetic moment** (*Evans*' method, d_8-THF): μ_{eff} = 1.11 μ_B. **EPR** (THF, 298 K): g_{iso} = 2.011, a(^{14}N, 2N) = 8.6 MHz. **UV/VIS/NIR** (THF, 298 K): λ_{abs} (ε) = 266 (120007), 298 (70582), 364 (92139), 601 (17899) nm ($Lmol^{-1}cm^{-1}$). **IR** (ATR [cm^{-1}]): ν = 3063 (vw), 2958 (m), 2896 (m), 2864 (m), 2824 (vw), 1639 (vw), 1574 (vw), 1557 (vw), 1466 (m), 1451 (m), 1398 (w), 1383 (w), 1350 (m); 1330 (w), 1282 (w), 1248 (w), 1206 (w), 1105 (vs), 1058 (s), 996 (w), 963 (s), 943 (s), 920 (s), 858 (m), 792 (m), 750 (m), 726 (m), 704 (m), 642 (w), 551 (vw), 551 (w), 531 (w), 495 (w), 469 (w).

Synthesis of [K(18-crown-6)(IMes-CS_2)] (2c)

KC_8 (35.5 mg, 262.7 *µ*mol, 1.0 eq.) and 18-crown-6 (69.5 mg, 262.8 *µ*mol, 1.0 eq.) was added to a suspension of IMes-CS_2 (100.0 mg, 262.8 *µ*mol, 1.0 eq.) in THF (10 mL). The mixture was stirred at room temperature for 48 hours and the purple solution was separated from undissolved solids by filtration through a glass wool filter. The residual solids were extracted with THF (3 x 10 mL) and the combined THF-fractions were reduced to approximately 30% of their volume by evaporation *in vacuo*. *n*-Hexane was added (10 mL) and the precipitate was collected by filtration and washed with *n*-hexane (3 x 5 mL) to yield [K(18-crown-6)(IMes-CS_2)] (**2c**) as a purple solid. Single crystals of **2c** suitable for X-ray diffraction were obtained by slow evaporation of a saturated solution of the product in MeCN at –30 °C. **Yield**: 42% (76.0 mg, 111.1 *µ*mol). **Elemental analysis**: $C_{40}H_{60}KN_2O_6S_2$ [768.15 g/mol] found (calc.): C 57.40 (57.71), H 7.69 (7.07), N 3.16 (4.10), S 6.52 (9.37)%. **Magnetic moment** (*Evans*'

method, d_8-THF): μ_{eff} = 1.07 μ_B. **EPR** (MeCN, 298 K): g_{iso} = 2.011, a(^{14}N, 2N) = 7.9 MHz (2.8 G). **UV/VIS/NIR** (MeCN, 298 K): λ_{abs} = 566 nm. **IR** (ATR [cm^{-1}]): ν = 2879 (m), 2860 (m), 2743 (vw), 1602 (m), 1570 (m), 1487 (m), 1472 (m), 1459 (m), 1379 (w), 1350 (m), 1284 (w), 1250 (m), 1223 (w) 1101 (vs), 1051 (s), 992 (m), 962 (s), 930 (m), 838 (s), 755 (w), 724 (w), 689 (w), 573 (w), 530 (w), 486 (w), 413 (w).

Synthesis of [Mg(^{Dipp}NacNac)(cAAC^{Me}-CS$_2$)] (3)

A solution of cAAC^{Me}-CS$_2$ (100.0 mg, 276.5 μmol, 2.0 eq.) in THF (5 mL) was added to a solution of [{Mg(^{Dipp}NacNac)}$_2$] (122.2 mg, 138.3 μmol, 1.0 eq.) in THF (5 mL) and stirred at room temperature for 18 hours. The solvent was removed *in vacuo* and the residue was extracted with *n*-hexane (15 mL) and separated from undissolved solids *via* filtration through a pad of celite. The filtrate was slowly evaporated at room temperature yielding [Mg(^{Dipp}NacNac)(cAAC^{Me}-CS$_2$)] (**3**) as a green crystalline solid. The single crystals obtained this way were suitable for X-ray diffraction. **Yield**: 42% (93.0 mg, 115.7 μmol). **Elemental analysis**: $C_{50}H_{72}MgN_3S_2$ [803.57 g/mol] found (calc.): C 74.08 (74.74), H 9.35 (9.03), N 5.24 (5.23), S 5.33 (7.98)%. **Magnetic moment** (*Evans*' method, C_6D_6): μ_{eff} = 1.20 μ_B. **EPR** (C_6H_6, 298 K): g_{iso} = 2.009, a(^{14}N, 1N) = 15.0 MHz. **UV/VIS/NIR** (C_6H_6, 298 K): λ_{abs} = 680 nm. **IR** (ATR [cm^{-1}]): ν = 3058 (w), 2959 (s), 2926 (m), 2866 (m), 1660 (m), 1623 (w), 1590 (w), 1546 (m), 1516 (m), 1457 (s), 1434 (s), 1400 (vs), 1362 (s), 1327 (s), 1314 (vs), 1254 (m), 1201 (m), 1173 (m), 1130 (w), 1101 (m), 1054 (m), 1040 (m), 1018 (s), 933 (m), 921 (m), 891 (w), 851 (w), 791 (s), 756 (s), 696 (w), 629 (vw), 577 (w), 521 (w), 437 (m), 406 (m).

3 NMR Section

3.1 General Information

NMR spectra were recorded at 298 K using a Bruker Avance 400 (^{1}H, 400.1 MHz; ^{13}C, 100.6 MHz) spectrometer. Chemical shifts (δ) are listed in parts per million (ppm) and were referenced *via* residual proton resonances of the deuterated solvent (C_6D_6: 7.16 ppm; $CDCl_3$: 7.26 ppm; d_8-THF: 1.72 ppm, 3.58 ppm; d_6-DMSO: 2.50 ppm), whereas ^{13}C{^{1}H} NMR spectra are reported relative to TMS using the natural-abundance carbon resonances (C_6D_6: 128.06 ppm; $CDCl_3$: 77.16 ppm; d_8-THF: 67.21 ppm, 25.31 ppm; d_6-DMSO: 39.52 ppm).[9] Spectra were plotted using the Mestre Nova software package.[10]

3.2 NMR Spectra

cAAC^{Me}-CS_2 (1a)

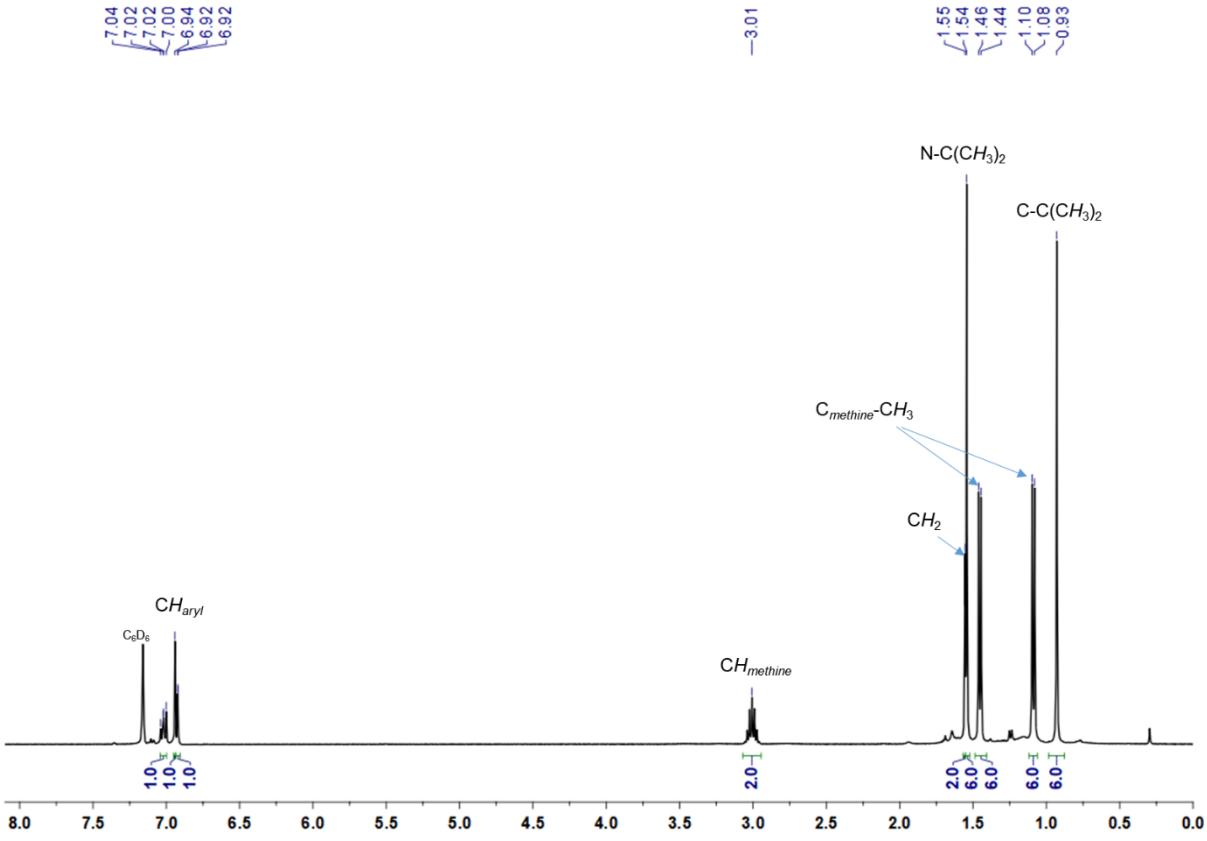


Figure S4. ^{1}H NMR spectrum of cAAC^{Me}-CS_2 (**1a**) in C_6D_6.

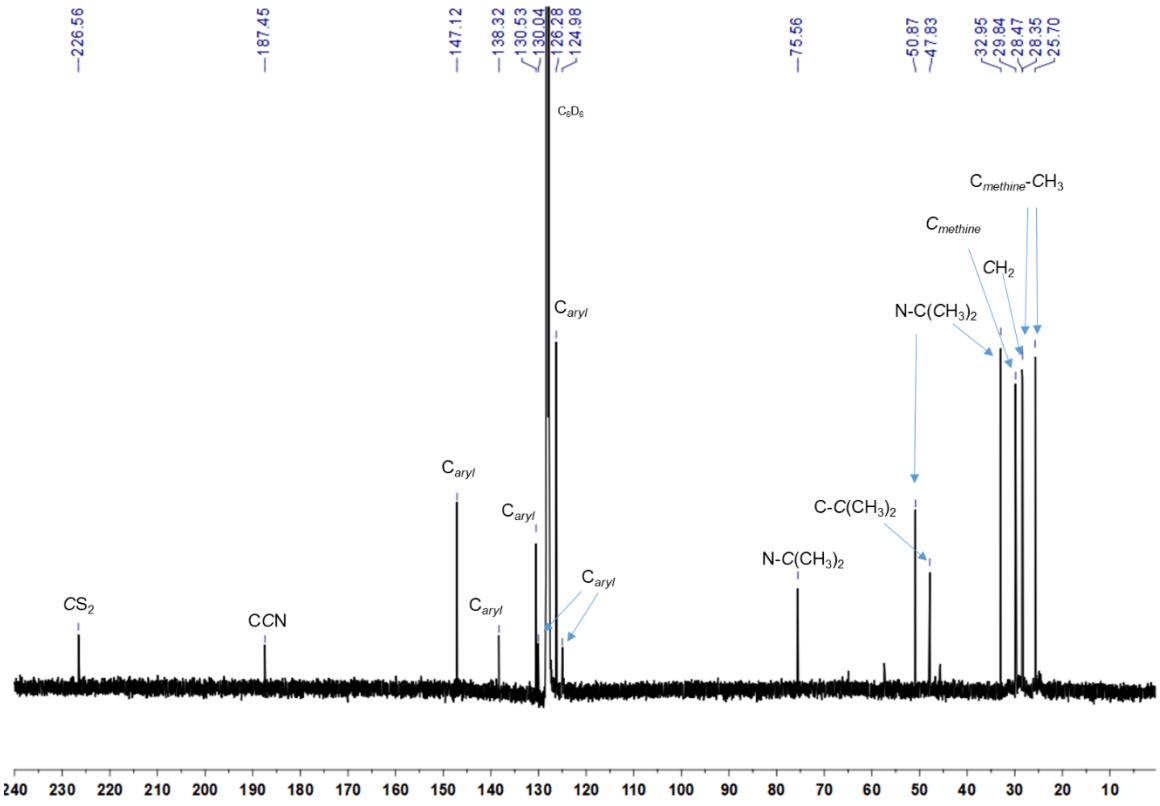


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of cAAC^{Me}-CS_2 (**1a**) in C_6D_6.

4 EPR Section

4.1 General Information

EPR measurements at X-band (9.38 GHz) were carried out using a Bruker ELEXSYS E580 CW EPR spectrometer equipped with an Oxford Instruments helium cryostat (ESR900) and a MercuryiTC temperature controller. The spectral simulations were performed using MATLAB 9.14.0.2206163 (R2023a) and the EasySpin 5.2.35 toolbox.[11]

4.2 EPR Spectra

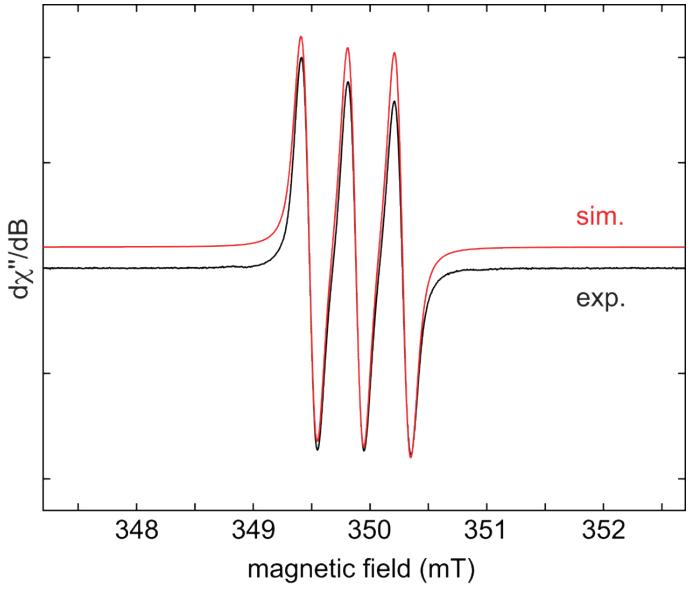


Figure S6. Experimental (black) and simulated (red) X-band EPR spectra of [K(18-crown-6)(cAAC^{Me}-CS_2)] (**2a**) in THF solution at room temperature. The EPR simulation involves an isotropic *g* factor of 2.013 and a nitrogen hyperfine coupling of $a(^{14}N)$ = 11.2 MHz (4.0 G).

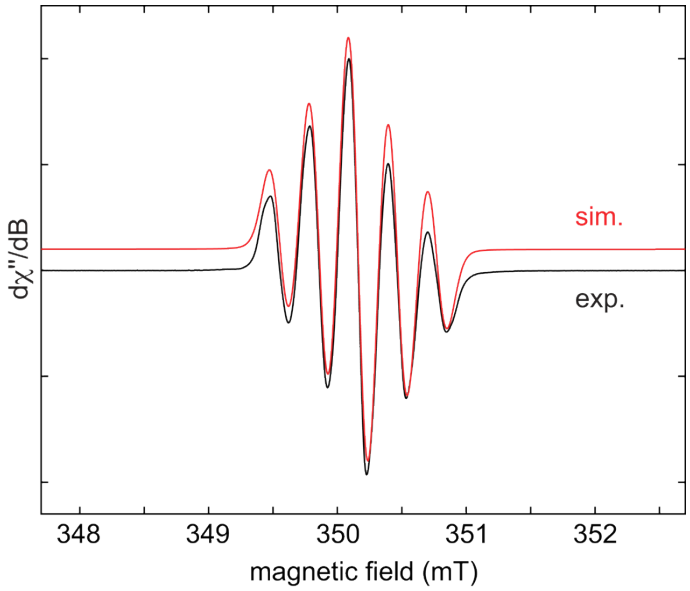


Figure S7. Experimental (black) and simulated (red) X-band EPR spectra of [K(18-crown-6)(IDipp-CS_2)] (**2b**) in THF solution at room temperature. The EPR simulation involves an isotropic *g* factor of 2.011 and a nitrogen hyperfine coupling of $a(^{14}N, 2N)$ = 8.6 MHz (3.05 G).

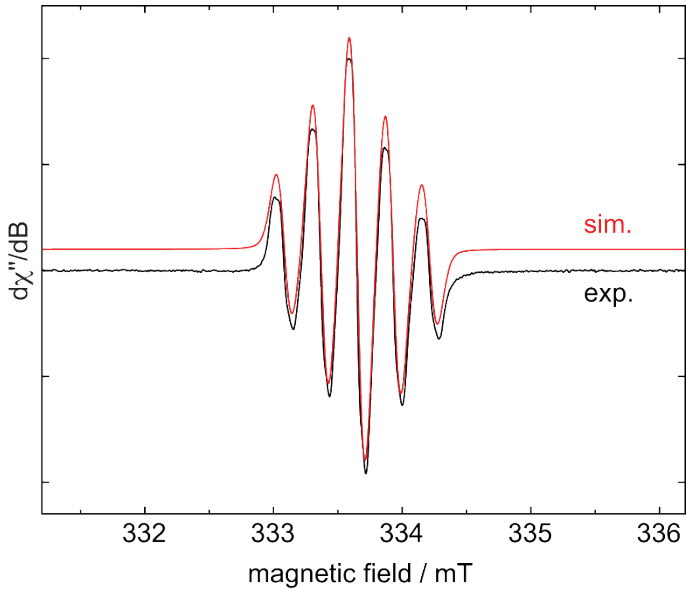


Figure S8. Experimental (black) and simulated (red) X-band EPR spectra of [K(18-crown-6)(IMes-CS_2)] (**2c**) in acetonitrile solution at room temperature. The EPR simulation involves an isotropic *g* factor of 2.011 and a nitrogen hyperfine coupling of $a(^{14}N, 2N)$ = 7.9 MHz (2.8 G).

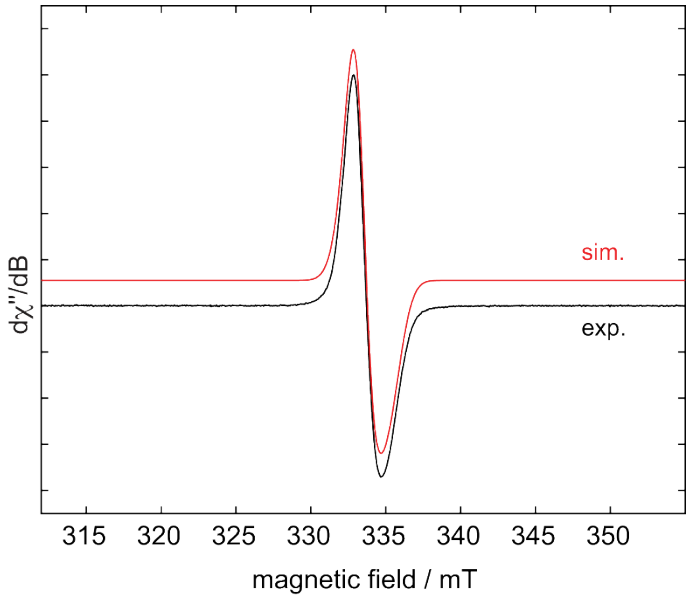


Figure S9. Experimental (black) and simulated (red) X-band EPR spectra of [K(18-crown-6)(IMes-CS_2)] (**2c**) in frozen acetonitrile solution at 70 K. The best-fit simulation parameters are: g_1 = 2.0136, g_2 = 2.0123, and g_3 = 2.0042 (average: g_{iso} = 2.0100).

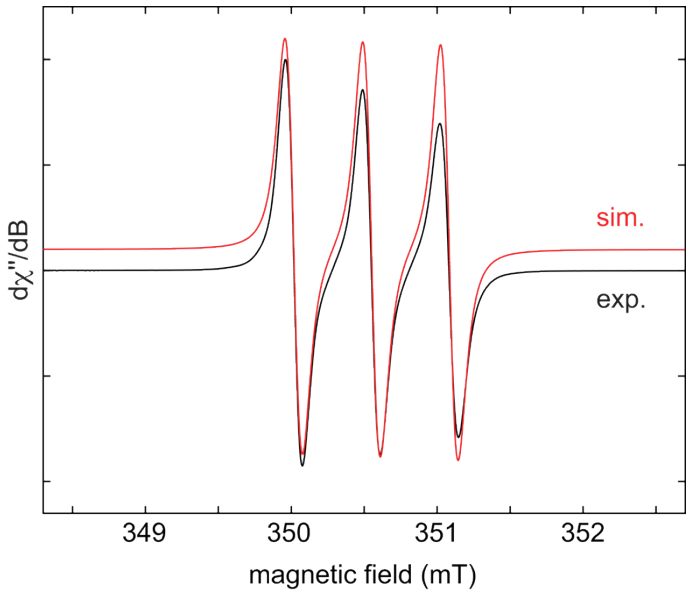


Figure S10. Experimental (black) and simulated (red) X-band EPR spectra of [Mg(^{Dipp}NacNac)(cAAC^{Me}-CS_2)] (**3**) in benzene solution at room temperature. The EPR simulation involves an isotropic *g* factor of 2.009 and a nitrogen hyperfine coupling of $a(^{14}N)$ = 15.0 MHz (5.3 G).

5 IR Section

5.1 General Information

Infrared spectra were recorded on a Bruker Alpha or Alpha II spectrometer as solids by using an ATR unit and plotted using the OPUS software package.[12]

5.2 IR Spectra

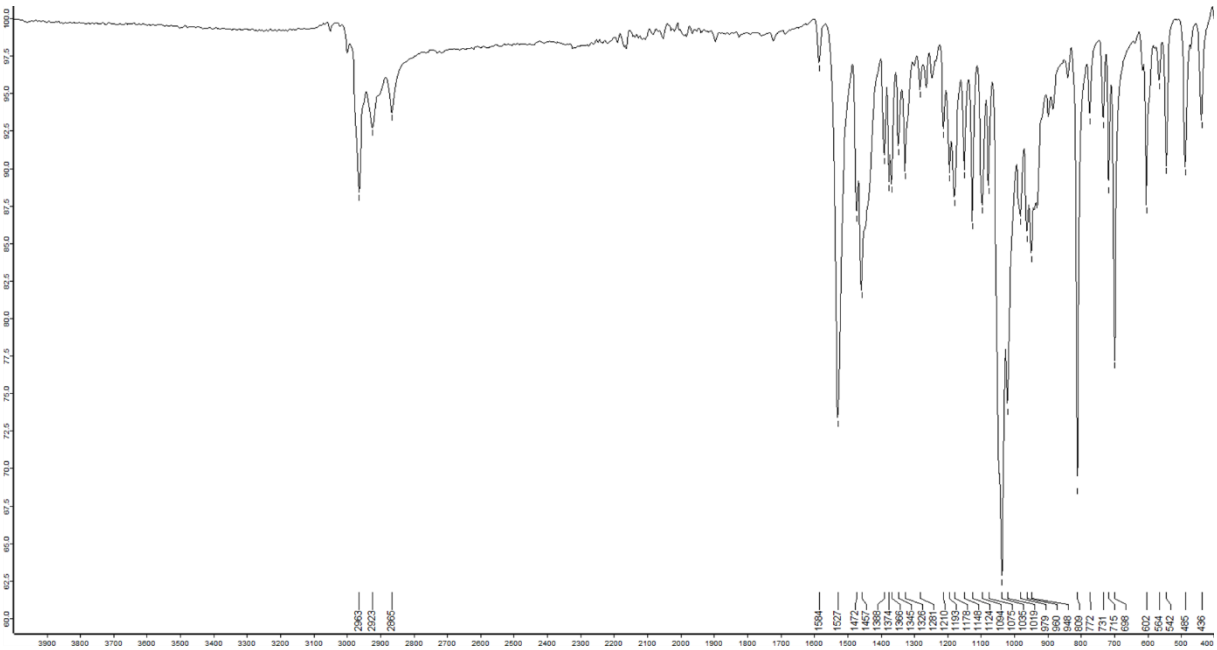


Figure S11. FT-IR spectrum (ATR) of cAAC^{Me}-CS_2 (**1a**).

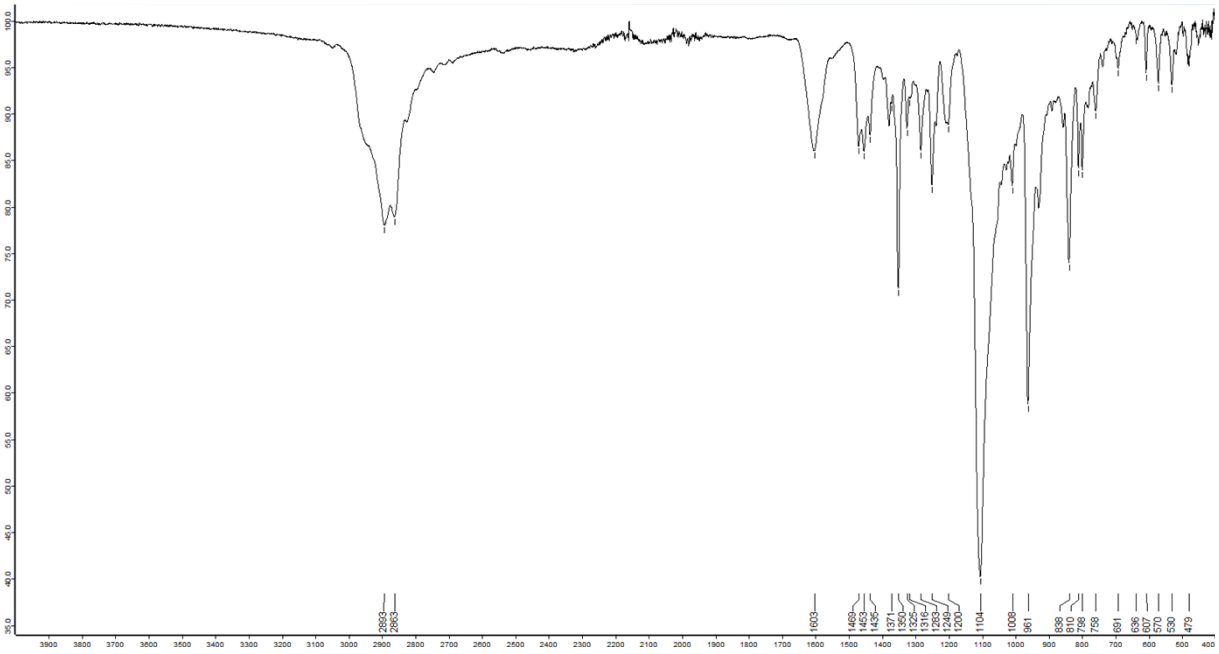


Figure S12. FT-IR spectrum (ATR) of [K(18-crown-6)(cAAC^{Me}-CS_2)] (**2a**).

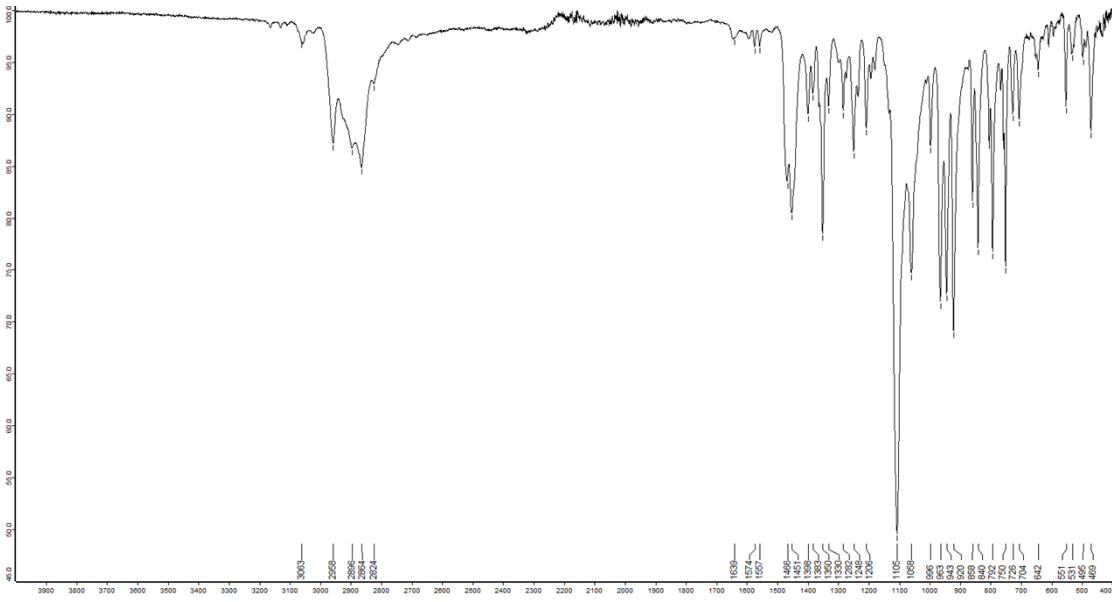


Figure S13. FT-IR spectrum (ATR) of [K(18-crown-6)(IDipp-CS_2)] (**2b**).

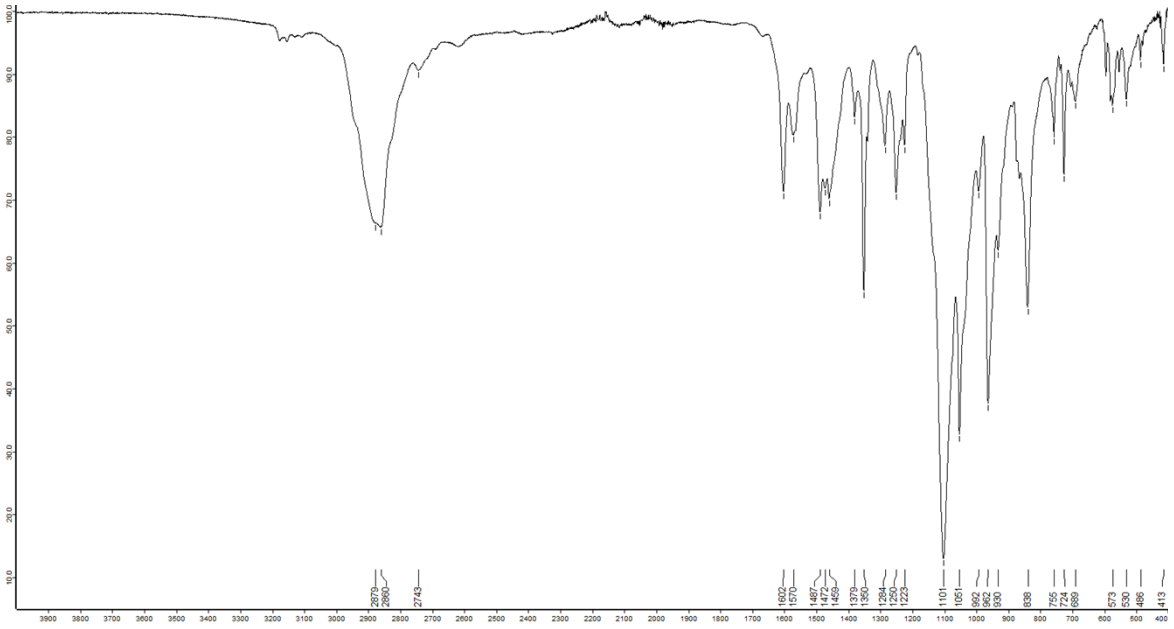


Figure S14. FT-IR spectrum (ATR) of [K(18-crown-6)(IMes-CS_2)] (**2c**).

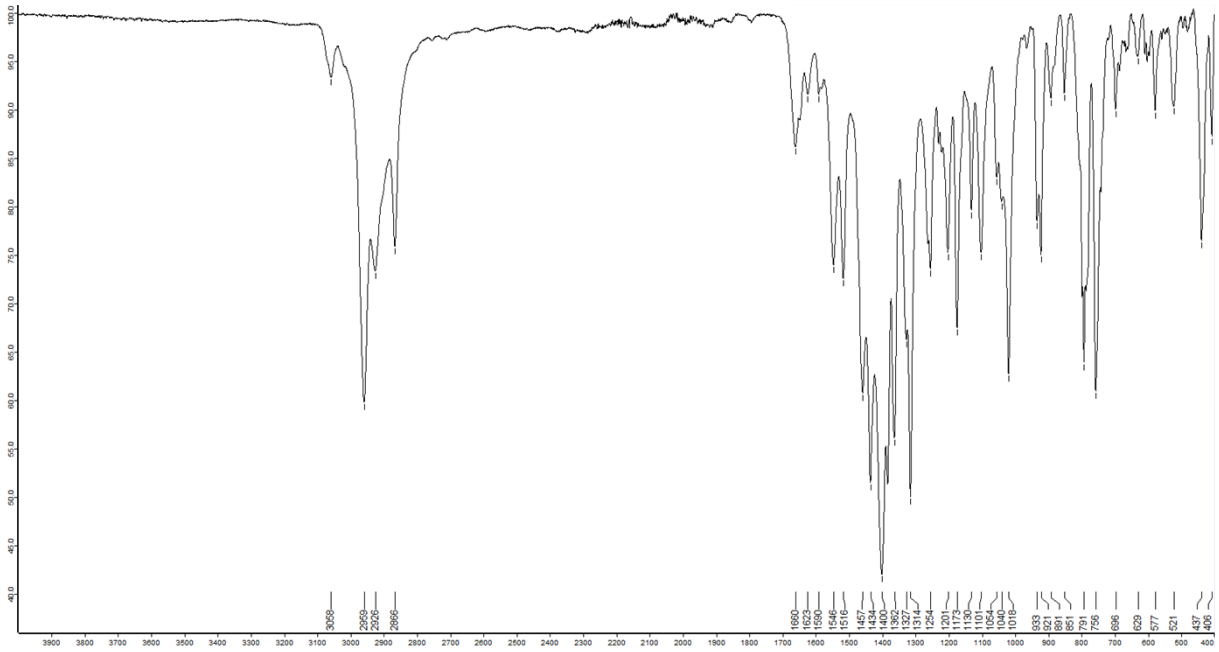


Figure S15. FT-IR spectrum (ATR) of [Mg(^{Dipp}NacNac)(cAAC^{Me}-CS_2)] (**3**).

6 Electrochemical Section

6.1 General Information

Cyclic voltammetry experiments were performed using a PINE Instruments AFCBP1 bipotentiostat or a Metrohm PGSTAT30 potentiostat with commercially available cells (ALS Co. Ltd., VC-4) in argon filled gloveboxes. The cells were used with a glassy carbon disc working electrode (2 mm diameter, BaSi) and a commercial platinum wire counter electrode (0.4 mm x 5.7 mm, ALS Co. Ltd.), as well as commercial silver wire reference electrodes separated from the main compartment by ion permeable porous glass (RE-7, ALS Co. Ltd.) and filled with a 0.01 M $AgNO_3$ stock solution in acetonitrile. Cyclovoltammetric measurements were performed with argon purged solvents. [TBA][PF_6] was obtained from Fluka (98%+) and used without further purification. All measurements were referenced against Ag^+/Ag as well as $[Fe(Cp)_2]^+$/$[Fe(Cp)_2]$ as an internal standard by addition of $[FeCp_2]$ at the end of the CV-experiment. The experiment control and recording were performed using the software packages AfterMath[13] or Nova[14], and data processing and plots were done with Origin 2023.[15]

6.2 Cyclovoltammograms

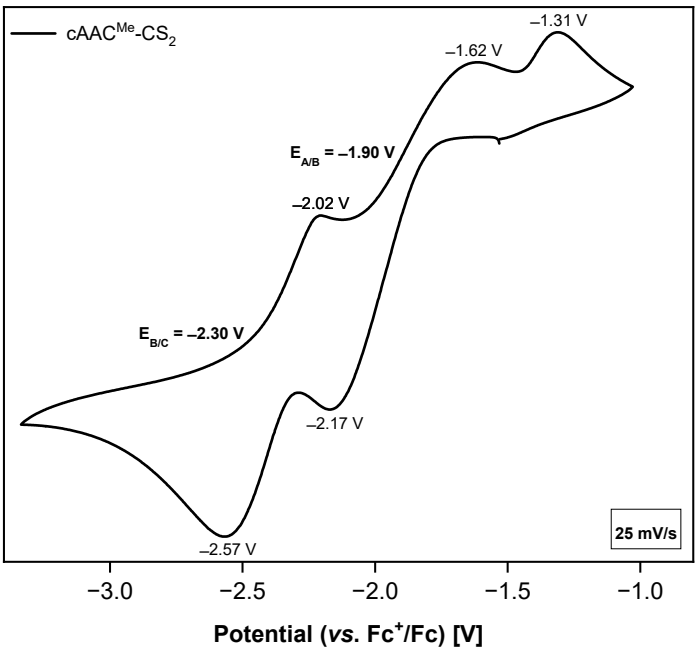


Figure S16. Cyclic voltammogram of cAAC^{Me}-CS_2 (**1a**) in THF using 0.1 M [TBA][PF_6] as supporting electrolyte at a scan rate of 25 mV/s. Potentials are referenced to the ferrocene/ferrocenium couple and the current is normalized to a value of 1.

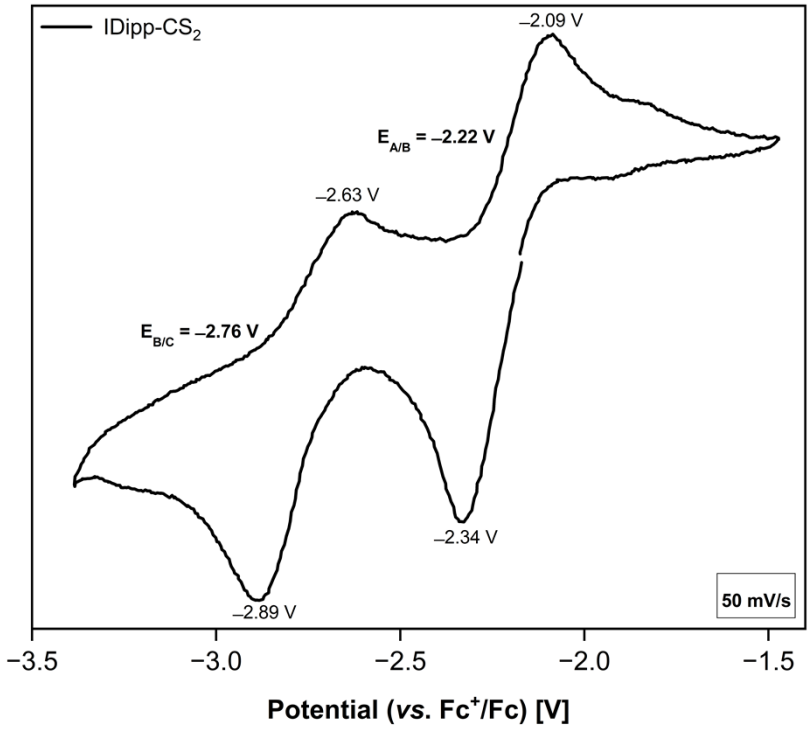


Figure S17. Cyclic voltammogram of IDipp-CS_2 (**1b**) in THF using 0.1 M [TBA][PF_6] as supporting electrolyte at a scan rate of 50 mV/s. Potentials are referenced to the ferrocene/ferrocenium redox couple and the current is normalized to a value of 1.

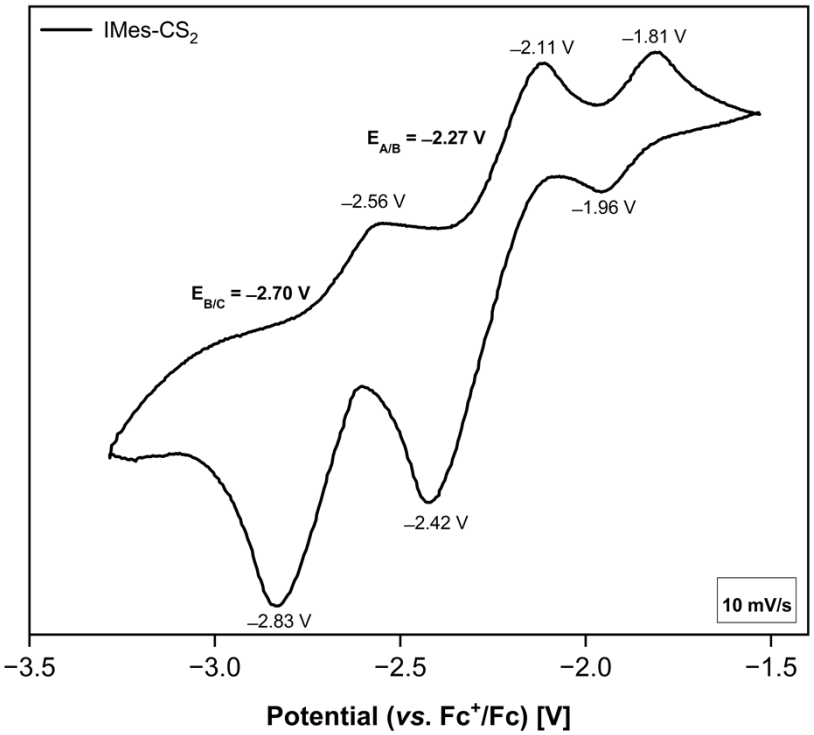


Figure S18. Cyclic voltammogram of IMes-CS_2 (**1c**) in THF using 0.1 M [TBA][PF_6] as supporting electrolyte at a scan rate of 10 mV/s. Potentials are referenced to the ferrocene/ferrocenium redox couple and the current is normalized to a value of 1.

7 UV/VIS/NIR Section

7.1 General Information

All measurements were performed in standard quartz cuvettes (1 cm x 1 cm cross-section) attached with a J. Young stopper under an argon atmosphere. Absorption spectra were recorded using a Perkin Elmer Lambda 465 or a Perkin Elmer Lambda 1050+ spectrophotometer. In the cases of **2a**, **2b** and **3**, rapid decomposition of the compounds forming the neutral adducts took place at low concentrations necessary for UV/VIS/NIR spectroscopy. Measurements were therefore performed in high concentrations with only the wavelength sections measured, in which the absorptions due to the radical characters of the coloured products were detected (450–1000 nm). Therefore, due to too high optical density at wavelengths below this range as well as overlapping with the decomposition products, absorptions thereof were not considered. Spectra were plotted using the Origin software package.[15]

7.2 UV/VIS/NIR Spectra

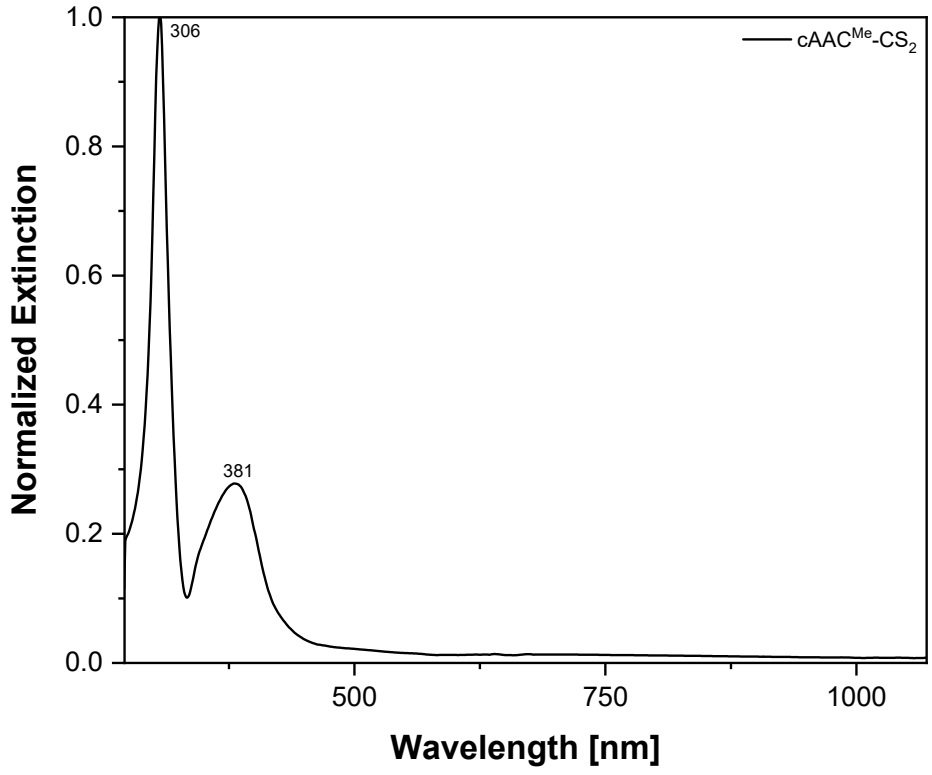


Figure S19. Absorption spectrum of $cAAC^{Me}$-CS_2 (**1a**) in benzene.

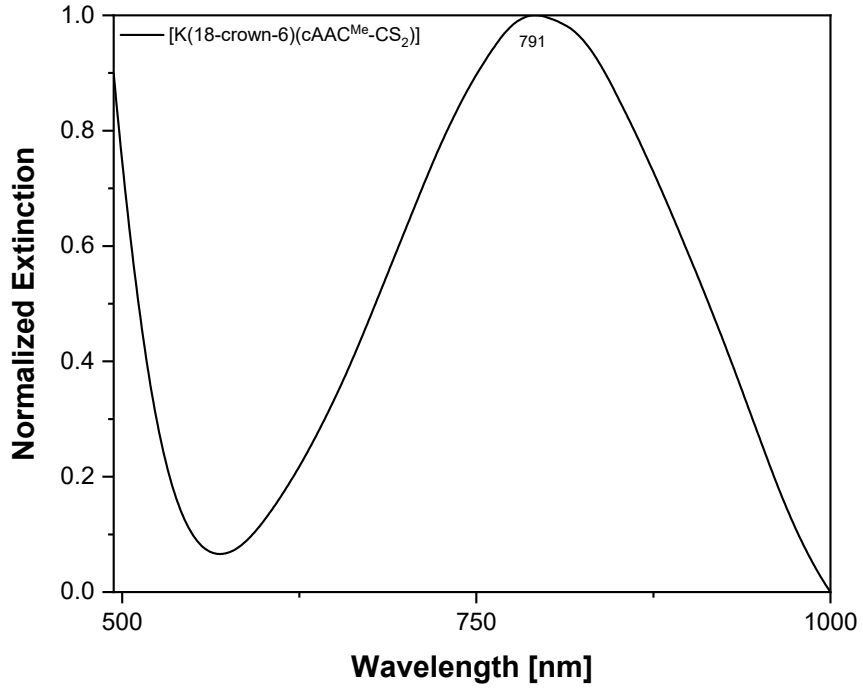


Figure S20. Absorption spectrum of [K(18-crown-6)(cAAC^{Me}-CS_2)] (**2a**) in benzene.

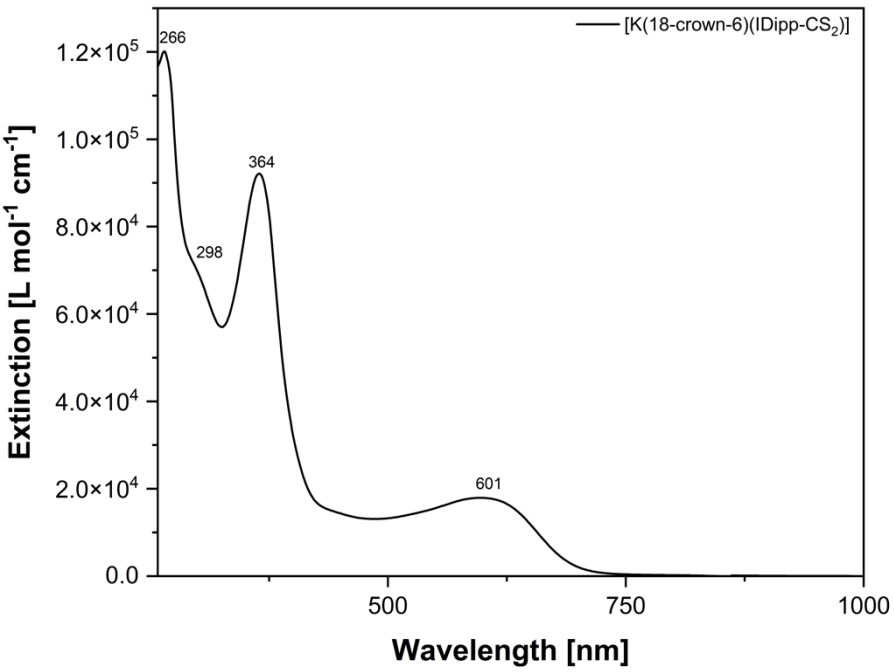


Figure S21. Absorption spectrum of [K(18-crown-6)(IDipp-CS_2)] (**2b**) in THF.

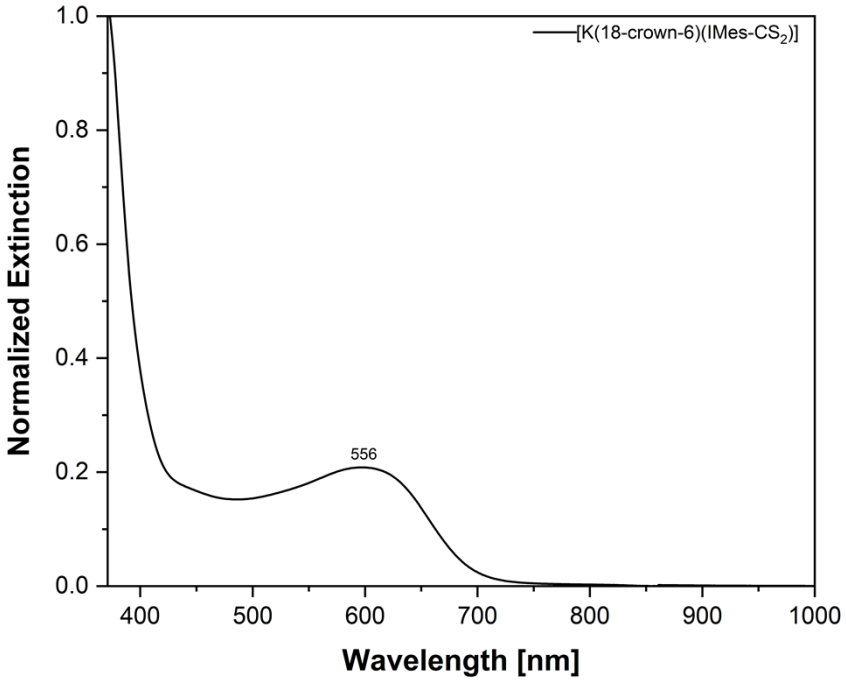


Figure S22. Absorption spectrum of [K(18-crown-6)(IMes-CS_2)] (**2c**) in MeCN.

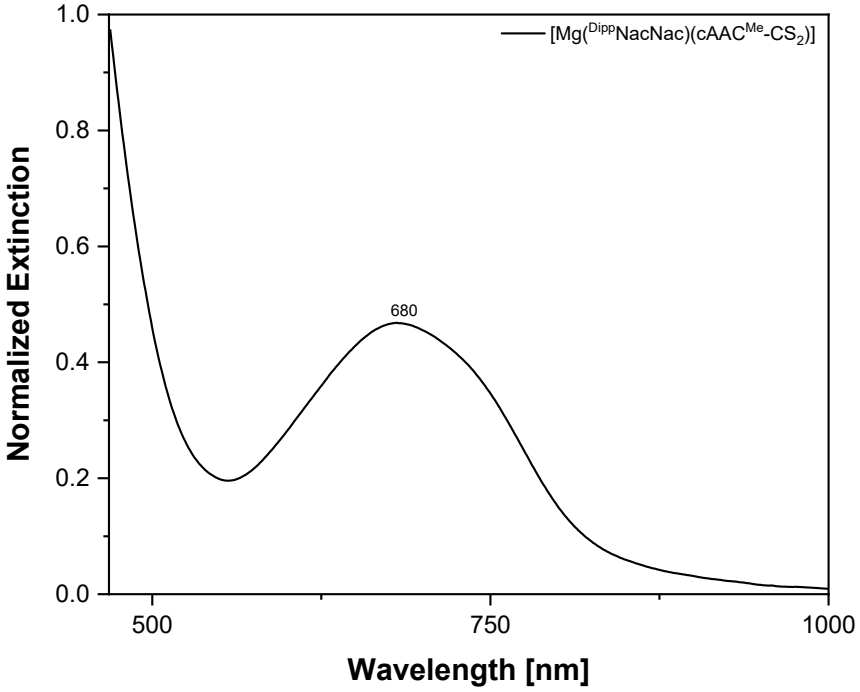


Figure S23. Absorption spectrum of [Mg(^{Dipp}NacNac)(cAAC^{Me}-CS_2)] (**3**) in benzene.

8 Crystallographic Section

8.1 General Information

Crystal data were either collected on a Rigaku XtaLAB Synergy-DW diffractometer with an HyPix-6000HE detector and monochromated CuK*α* or MoK*α* radition equipped with an Oxford Cryo 800 cooling unit or on a XtaLAB Synergy Dualflex HyPix diffractometer with a Hybrid Pixel array detector and multi-layer mirror monochromated CuK*α* radiation. The Crystals were immersed in a film of perfluoropoly-ether oil on a glass fiber MicroMount™ (MiTeGen) and data were collected at 100 K. The images were processed with the Bruker or Crysalis software packages and equivalent reflections were merged. Corrections for Lorentz-polarization effects and absorption were performed if necessary and the structures were solved by direct methods. Subsequent difference Fourier syntheses revealed the positions of all other non-hydrogen atoms. The structures were solved by using the ShelXTL software package. [16] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned to idealized positions and were included in structure factor calculations. Figures are created using Diamond Crystal and Molecular Structure Visualisation software.[17]

Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no.s CCDC 2390729 (**1a**), CCDC 2390730 (**3**), CCDC 2390731 (**2c**), CCDC 2390732 (**2b**), and CCDC 2390733 (**2a(THF)**). Copies of the data can be obtained free of charge on application to CCDC (https://www.ccdc.cam.ac.uk).

8.2 Crystal Data

Crystal Data for cAAC^{Me}-CS$_2$ (1a):

$C_{21}H_{31}NS_2$, M_r = 361.61 g/mol, T = 100.00(10) K, λ = 1.54184 Å, orange block, 0.160 × 0.140 × 0.070 mm^3, monoclinic, space group $P2_1$, a = 8.0364(2) Å, b = 14.9846(4) Å, c = 8.9999(3) Å, α = 90 °, β = 113.047(3) °, γ = 90 °, V = 997.28(5) Å^3, Z = 2, ρ_{calc} = 1.204 Mg/m^3, μ = 2.409 mm^{-1}, F(000) = 392, 7881 reflections, $-9 \le h \le 10$, $-18 \le k \le 16$, $-11 \le l \le 7$, 5.341 ° < θ < 77.647 °, completeness 97.6%, 3373 independent reflections, 3324 reflections observed with [$I > 2\sigma(I)$], 225 parameters, 1 restraint, R indices (all data) R_1 = 0.0337, wR_2 = 0.0884, final R indices [$I > 2\sigma(I)$] R_1 = 0.0334, wR_2 = 0.0881, largest difference peak and hole 0.335 and –0.274 e Å^{-3}, Goof = 1.041.

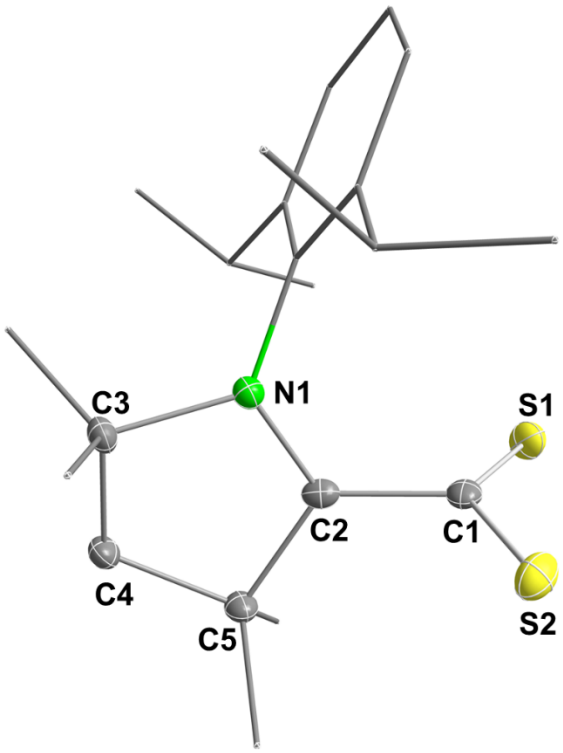


Figure S24. Molecular structure of cAAC^{Me}-CS$_2$ (**1a**) in the solid-state (ellipsoids set at 50% probability level). The hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: S1–C1 1.653(3), S2–C1 1.681(3), C1–C2 1.485(3), C2–C5 1.523(3), C2–N1 1.307(3), N1–C3 1.540(3), C3–C4 1.523(4), C4–C5 1.553(3), ∢S1C1S2 131.0(1), ∢N1C2C1S1 83.7(3).

Crystal Data for [K(THF)(18-crown-6)(cAAC^{Me}-CS$_2$)] (2a):

$C_{37}H_{63}KNO_7S_2$, M_r = 737.10 g/mol, T = 100.00(10) K, λ = 1.54184 Å, green block, 0.130 × 0.090 × 0.060 mm^3, monoclinic, space group $P2_1/n$, a = 17.1497(2) Å, b = 10.44560(10) Å, c = 23.0760(2) Å, α = 90 °, β = 100.7780(10) °, γ = 90 °, V = 4060.89(7) Å^3, Z = 4, ρ_{calc} = 1.206 Mg/m^3, μ = 2.459 mm^{-1}, $F(000)$ = 1596, 39466 reflections, –20 ≤ h ≤ 21, –13 ≤ k ≤ 12, –29 ≤ l ≤ 27, 2.961 ° < θ < 77.468 °, completeness 99.3%, 8338 independent reflections, 7283 reflections observed with [$I > 2\sigma(I)$], 487 parameters, 214 restraints, R indices (all data) R_1 = 0.0661, wR_2 = 0.1659, final R indices [$I > 2\sigma(I)$] R_1 = 0.0594, wR_2 = 0.1609, largest difference peak and hole 1.212 and –1.210 e Å^{-3}, Goof = 1.039.

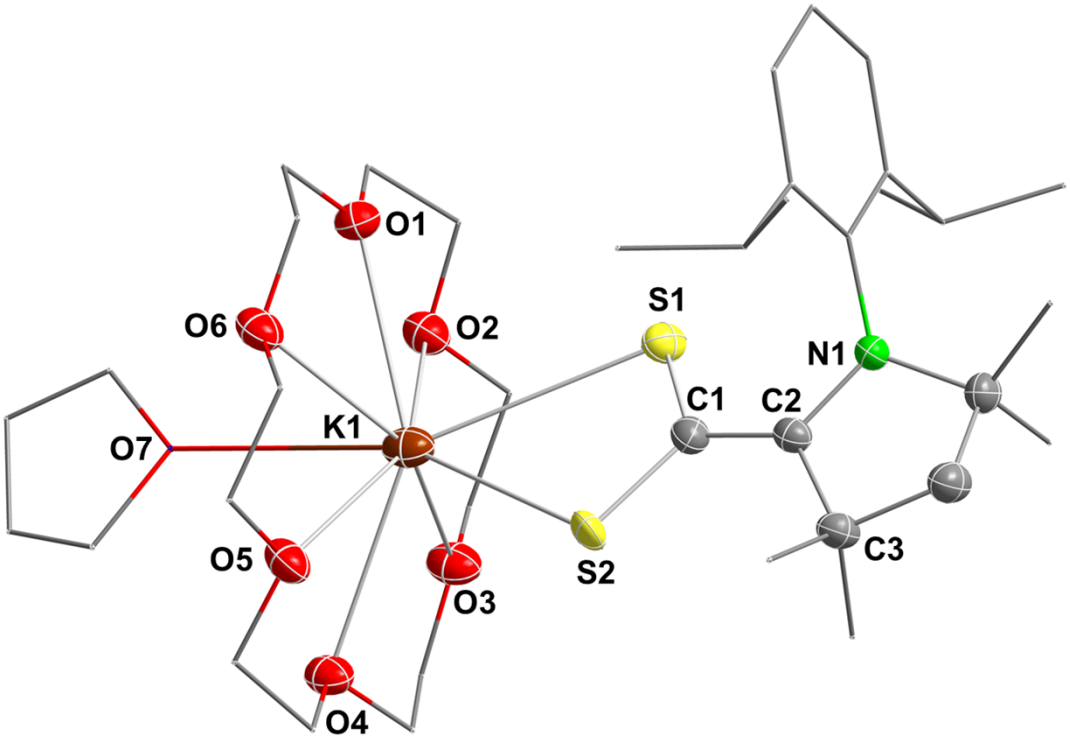


Figure S25. Molecular structure of [K(THF)(18-crown-6)(cAAC^{Me}-CS$_2$)] (**2a**): in the solid-state (ellipsoids set at 50% probability level). The hydrogen atoms are omitted for clarity. As the structure contained a two-fold disorder (43:57) of the THF molecules only the part of 57% occupancy is shown. Selected bond lengths [Å] and angles [°]: S1–K1 3.116(1), S2–K1 3.351(1), K1–O1 2.831(2), K1–O2 2.966(2), K1–O3 2.829(2), K1–O4 2.946(2), K1–O5 2.784(2), K1–O6 2.946(2), K1–O7 3.320(5), S1–C1 1.728(2), S2–C1 1.723(3), C1–C2 1.410(3), C2–N1 1.393(3), ∡S1C1S2 117.9(1), ∡N1C2C1S1 10.9(3).

Crystal Data for [K(18-crown-6)(IDipp-CS_2)]·(18-crown-6) (2b·18-crown-6):

$C_{50.3}H_{80.86}K_{0.87}N_2O_{11.21}S_2$, M_r = 992.69 g/mol, T = 100.00(10) K, λ = 1.54184 Å, black plate, 0.280 × 0.180 × 0.080 mm³, triclinic, space group $P\bar{1}$, a = 12.4442(3) Å, b = 12.7336(4) Å, c = 18.2742(6) Å, α = 89.060(2) °, β = 78.915(2) °, γ = 80.742(2) °, V = 2804.36(15) Å³, Z = 2, ρ_{calc} = 1.176 Mg/m³, μ = 1.886 mm⁻¹, F(000) = 1114, 49723 reflections, –14 ≤ h ≤ 14, –15 ≤ k ≤ 15, –21 ≤ l ≤ 21, 2.464 ° < θ < 67.071 °, completeness 99.1%, 9921 independent reflections, 8176 reflections observed with [$I > 2\sigma(I)$], 632 parameters, 1453 restraints, R indices (all data) R_1 = 0.1315, wR_2 = 0.3140, final R indices [$I > 2\sigma(I)$] R_1 = 0.1159, wR_2 = 0.3022, largest difference peak and hole 1.521 and –1.642 e Å⁻³, Goof = 1.058.

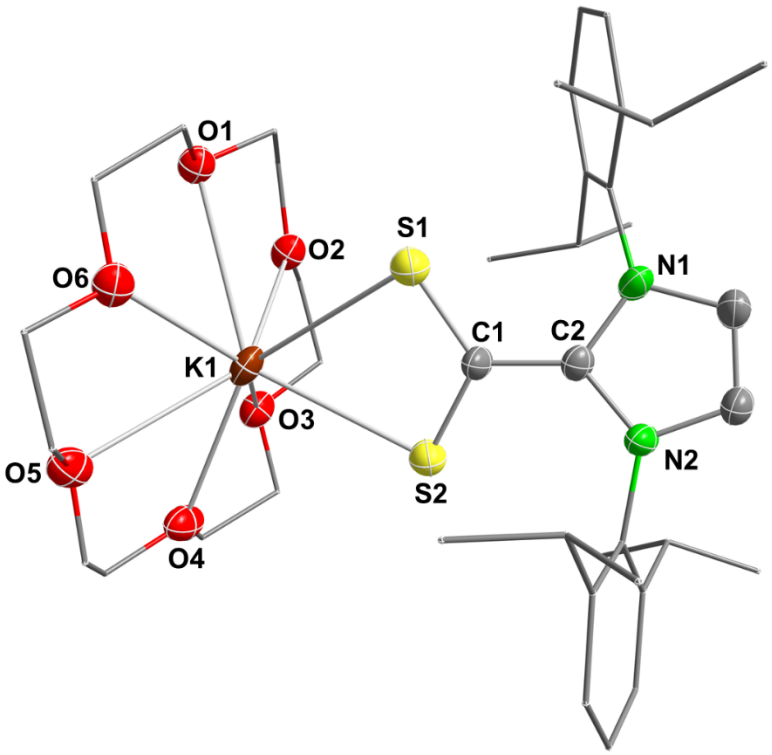


Figure S26. Molecular structure of [K(18-crown-6)(IDipp-CS_2)]·(18-crown-6) (**2b·18-crown-6**) in the solid-state (ellipsoids set at 50% probability level). Due to rapid decomposition of compound **2b** the obtained structure is of a co-crystal of **2b·18-crown-6** and 13.1% oxidized, neutral IDipp-CS_2 (**1b**). The hydrogen atoms as well as one molecule of co-crystallized 18-crown-6 and the partially co-crystallized IDipp-CS_2 were omitted for clarity. Selected bond lengths [Å] and angles [°]: K1–O1 2.960(1), K1–O2 2.812(1), K1–O3 2.993(1), K1–O4 2.836(1), K1–O5 3.079(1), K1–O6 2.963(1), C1–C2 1.415(1), C2–N1 1.375(1), C2–N2 1.386(1), S1–C1 1.709(1), S2–C1 1.737(9), S1–K1 3.221(1), S2–K1 3.247(1), ∡N1C2C1S1 29.1(1), ∡N2C2C1S2 31.3(1), ∡S1C1S2 124.0(2).

Crystal Data for [K(18-crown-6)(IMes-CS_2)]·2MeCN (2c·2MeCN):

$C_{38}H_{54}KN_4O_6S_2$, M_r = 766.07 g/mol, T = 100.00(10) K, λ = 1.54184 Å, purple block, 0.300 × 0.080 × 0.080 mm^3, monoclinic, space group $P2_1/n$, a = 8.95410(10) Å, b = 15.7437(3) Å, c = 28.9534(5) Å, α = 90 °, β = 96.571(2) °, γ = 90 °, V = 4054.77(11) $Å^3$, Z = 4, ρ_{calc} = 1.255 Mg/m^3, μ = 2.497 mm^{-1}, $F(000)$ = 1636, 37237 reflections, $-10 \le h \le 8$, $-18 \le k \le 18$, $-34 \le l \le 33$, 3.073 ° < θ < 67.080 °, completeness 99.8%, 7239 independent reflections, 5918 reflections observed with [$I > 2\sigma(I)$], 468 parameters, 0 restraints, R indices (all data) R_1 = 0.0843, wR_2 = 0.2076, final R indices [$I > 2\sigma(I)$] R_1 = 0.0734, wR_2 = 0.1994, largest difference peak and hole 0.823 and –0.815 e $Å^{-3}$, Goof = 1.093.

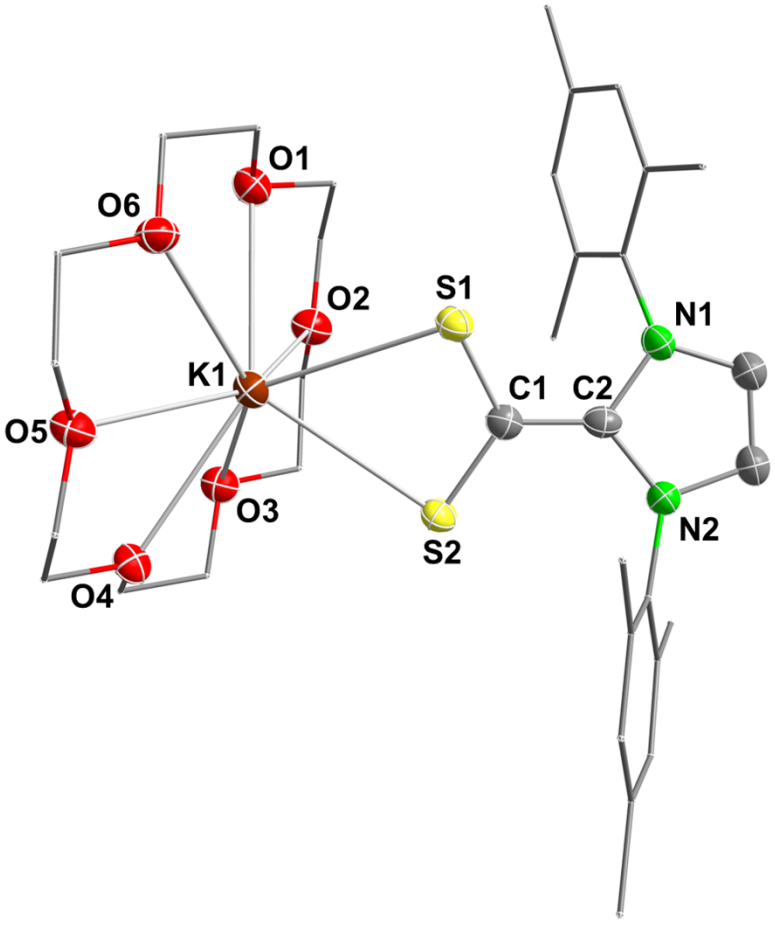


Figure S27. Molecular structure of [K(18-crown-6)(IMes-CS_2)]·2MeCN (**2c·2MeCN**) in the solid-state (ellipsoids set at 50% probability level). The hydrogen atoms as well as two molecules of co-crystallized MeCN were omitted for clarity. Selected bond lengths [Å] and angles [°]: K1–O1 3.017(2), K1–O2 2.806(2), K1–O3 3.01(2), K1–O4 2.991(2), K1–O5 2.931(2), K1–O6 2.942(2), C1–C2 1.407(5), C2–N1 1.388(4), C2–N2 1.387(4), S1–C1 1.734(3), S2–C1 1.733(3), S1–K1 3.216(1), S2–K1 3.212(8), ∡N1C2C1S1 31.2(4), ∡N2C2C1S2 31.8(4), ∡S1C1S2 124.0(2).

Crystal Data for [Mg(^{Dipp}NacNac)(cAAC^{Me}-CS_2)] (3):

$C_{50}H_{72}MgN_3S_2$, M_r = 803.54 g/mol, T = 100.00(10) K, λ = 0.71073 Å, green plate, 0.450 × 0.340 × 0.120 mm^3, monoclinic, space group $P2_1/m$, a = 10.6763(2) Å, b = 19.9981(3) Å, c = 11.7538(2) Å, α = 90 °, β = 109.747(2) °, γ = 90 °, V = 2361.93(7) Å^3, Z = 2, ρ_{calc} = 1.130 Mg/m^3, μ = 0.162 mm^{-1}, F(000) = 874, 46455 reflections, $-13 \le h \le 13$, $-26 \le k \le 24$, $-14 \le l \le 15$, 1.841 ° < θ < 28.837 °, completeness 99.9%, 5611 independent reflections, 5611 reflections observed with [$I > 2\sigma(I)$], 280 parameters, 0 restraints, R indices (all data) R_1 = 0.0434, wR_2 = 0.1050, final R indices [$I > 2\sigma(I)$] R_1 = 0.0388, wR_2 = 0.1020, largest difference peak and hole 0.410 and –0.439 e Å^{-3}, Goof = 1.041.

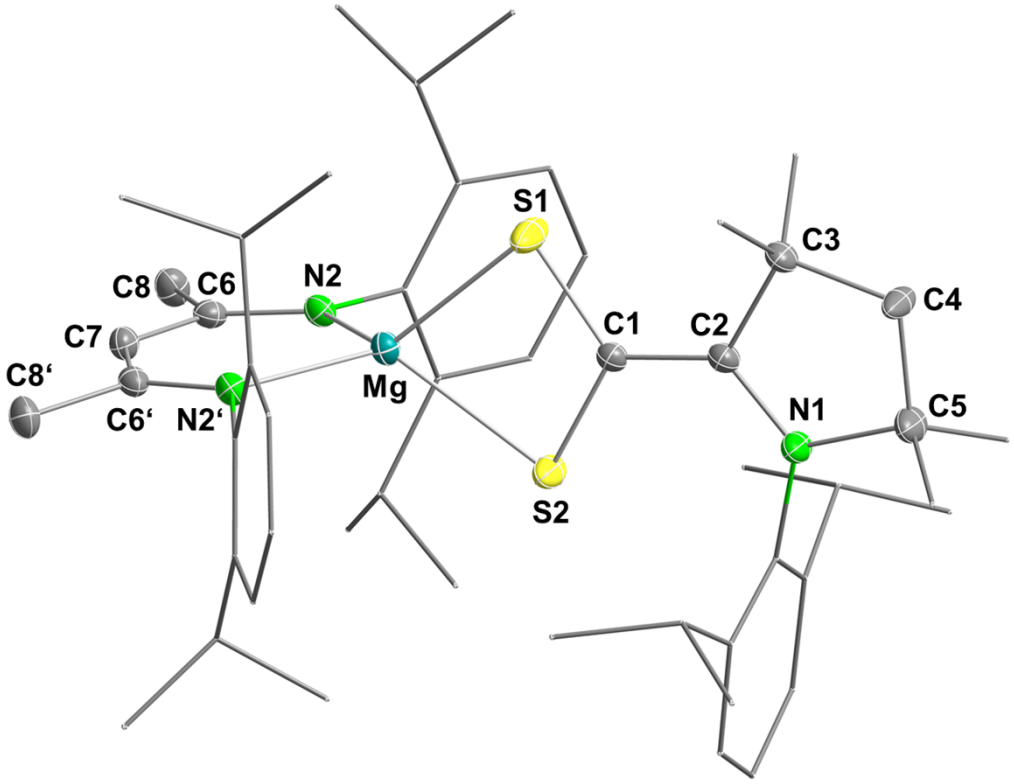


Figure S28. Molecular structure of [Mg(^{Dipp}NacNac)(cAAC^{Me}-CS_2)] (**3**) in the solid-state (ellipsoids set at 50% probability level). The hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Mg–S1 2.443(1), Mg–S2 2.430(1), Mg–N2 2.029(1), S1–C1 1.736(2), S2–C1 1.727(2), C1–C2 1.420(2), N1–C2 1.358(2), ∡S1C1S2 115.8(1), ∡N2MgN2’ 92.9(1), ∡S1MgS2 74.1(1), ∡S1MgN2 124.8(1), ∡S2MgN2 121.9(1), ∡N1C2C1S2 0.0(2).

9 Quantumchemical Calculations Section

9.1 General Information

Calculations were carried out using the TURBOMOLE V7.8 program suite, a development of the University of Karlsruhe and the Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from https://www.turbomole.org.[18] Geometry optimizations and frequency calculations were performed using (RI-)DFT calculations[19] on a m4 grid employing the BP86[20] functional and def2-SVP basis sets.[21] Vibrational frequencies were calculated at the same level with the AOFORCE[22] module and all structures represented true minima without imaginary frequencies (denoted as BP86/def2-SVP). Total energies, orbital energies, and orbital plots and were calculated using these geometries, the B3LYP[20b,21] functional and a def2-TZVP[21] basis set for all atoms (denoted as B3LYP/def2-TZVP). Vertical excitation energies were computed at the TD-DFT level[24] using the long range corrected *ω*B97X-D[25] functional and a def2-TZVP basis set (denoted as *ω*B97X/def2-TZVP).

9.2 Cartesian Coordinates of Geometry-optimized Molecules

IMe^{Me}-CS$_2$_C2v_planar
Energy = -1217.515793033

C	0.0000000	0.0000000	1.3428718
N	0.0000000	1.0944320	0.4921197
C	0.0000000	0.6888145	-0.8379725
N	0.0000000	-1.0944320	0.4921197
C	0.0000000	-0.6888145	-0.8379725
C	0.0000000	2.5309377	0.7919232
H	0.0000000	2.6471595	1.8977792
C	0.0000000	-2.5309377	0.7919232
H	0.0000000	-2.6471595	1.8977792
C	0.0000000	0.0000000	2.8585308
S	0.0000000	-1.4762730	3.7147432
S	0.0000000	1.4762730	3.7147432
C	0.0000000	-1.6497253	-1.9802770
H	0.8924117	-2.3092841	-1.9693077
H	-0.8924117	-2.3092841	-1.9693077
H	0.0000000	-1.1014281	-2.9401285
C	0.0000000	1.6497253	-1.9802770
H	-0.8924117	2.3092841	-1.9693077
H	0.8924117	2.3092841	-1.9693077
H	0.0000000	1.1014281	-2.9401285
H	0.9036950	2.9937828	0.3498290
H	-0.9036950	2.9937828	0.3498290
H	-0.9036950	-2.9937828	0.3498290
H	0.9036950	-2.9937828	0.3498290

IMe^{Me}-CS$_2$_C2v_orthogonal
Energy = -1217.532315188

C	0.0000000	0.0000000	1.2551939
N	0.0000000	1.0926631	0.4450001
C	0.0000000	0.6902504	-0.8987000
N	0.0000000	-1.0926631	0.4450001
C	0.0000000	-0.6902504	-0.8987000
C	0.0000000	2.4670128	0.9239584
H	0.0000000	2.4512276	2.0279766
C	0.0000000	-2.4670128	0.9239584
H	0.0000000	-2.4512276	2.0279766
C	0.0000000	0.0000000	2.7407539
S	1.5571679	0.0000000	3.3993486
S	-1.5571679	0.0000000	3.3993486
C	0.0000000	-1.6709060	-2.0238954
H	0.8944455	-2.3290320	-2.0021508
H	-0.8944455	-2.3290320	-2.0021508
H	0.0000000	-1.1426033	-2.9952245
C	0.0000000	1.6709060	-2.0238954
H	-0.8944455	2.3290320	-2.0021508
H	0.8944455	2.3290320	-2.0021508
H	0.0000000	1.1426033	-2.9952245
H	0.9042666	3.0005529	0.5704574
H	-0.9042666	3.0005529	0.5704574
H	-0.9042666	-3.0005529	0.5704574
H	0.9042666	-3.0005529	0.5704574

IMe^{Me}-CS$_2$
Energy = -1217.532314686

C	-0.0004594	-0.0000000	1.0197395
N	-0.0007070	1.0926653	0.2094828
C	-0.0016693	0.6902812	-1.1341414
N	-0.0007070	-1.0926653	0.2094828
C	-0.0016693	-0.6902812	-1.1341414
C	-0.0006089	2.4670097	0.6884218
H	-0.0031368	2.4511802	1.7924889
C	-0.0006089	-2.4670097	0.6884218
H	-0.0031368	-2.4511802	1.7924889
C	0.0015882	-0.0000000	2.5053355
S	1.5597911	-0.0000000	3.1617547
S	-1.5544833	0.0000000	3.1661126
C	0.0000780	-1.6708488	-2.2593880
H	0.8950092	-2.3282959	-2.2368488
H	-0.8938246	-2.3297431	-2.2385562
H	0.0005243	-1.1425591	-3.2307198
C	0.0000780	1.6708488	-2.2593880
H	-0.8938246	2.3297431	-2.2385562
H	0.8950092	2.3282959	-2.2368488
H	0.0005243	1.1425591	-3.2307198
H	0.9048729	2.9999432	0.3367992
H	-0.9037561	3.0011376	0.3328402
H	-0.9037561	-3.0011376	0.3328402
H	0.9048729	-2.9999432	0.3367992

$[IMe^{Me}\text{-}CS_2]^-$

Energy = -1217.542922891

C	0.0000188	0.0000110	1.0988969
N	-0.1479335	1.1080123	0.2257897
C	-0.0794491	0.6825525	-1.1069669
N	0.1480265	-1.1079948	0.2258063
C	0.0795225	-0.6825552	-1.1069548
C	0.0489910	2.4875297	0.6238020
H	-0.3603154	2.5807222	1.6640268
C	-0.0488821	-2.4875092	0.6238258
H	0.3604036	-2.5806817	1.6640584
C	-0.0000989	0.0000136	2.5363934
S	0.9280481	-1.2181800	3.3821323
S	-0.9283725	1.2182106	3.3819698
C	0.1582254	-1.6344345	-2.2555824
H	1.1140328	-2.2061036	-2.2631066
H	-0.6603032	-2.3893454	-2.2432271
H	0.0918683	-1.0876540	-3.2164802
C	-0.1582739	1.6343998	-2.2556167
H	-1.1141224	2.2060047	-2.2630977
H	0.6602043	2.3893676	-2.2433283
H	-0.0919372	1.0876015	-3.2165060
H	1.1300057	2.7698661	0.6268585
H	-0.4951585	3.1620624	-0.0679491
H	-1.1298896	-2.7698623	0.6268717
H	0.4952893	-3.1620330	-0.0679158

$cAAC^{Me}\text{-}CS_2$

Energy = -1669.278163662

C	0.7837347	-0.3763069	0.9292061
C	0.4586703	0.3992543	2.2230311
C	0.4253847	1.8703853	1.7055522
C	1.1627868	1.8843880	0.3479050
H	-0.6253316	2.1927962	1.5544003
H	0.8860023	2.5746221	2.4250488
C	-0.9421071	-0.0520203	2.7119649
H	-1.7058028	0.0348102	1.9143613
H	-0.9271068	-1.1069730	3.0468451
H	-1.2532842	0.5863764	3.5649147
C	1.4633809	0.2058197	3.3771523
H	1.5223324	-0.8570673	3.6782588
H	2.4846075	0.5282923	3.1006861
H	1.1284647	0.8034515	4.2506062
C	0.6295351	2.9395961	-0.6212487
H	0.8851958	3.9439450	-0.2286661
H	1.0909388	2.8420864	-1.6238143
H	-0.4682804	2.8921295	-0.7334142
C	2.6812338	2.0779599	0.5354350
H	3.2084671	2.1079051	-0.4360916
H	2.8664876	3.0431804	1.0482801
H	3.1252949	1.2671774	1.1450856
N	0.8888101	0.4530362	-0.1197950
C	0.7435181	0.0675853	-1.5191490
C	-0.5634351	0.1426429	-2.0961754
C	1.8650654	-0.3552219	-2.2877338
C	-0.7075453	-0.2109076	-3.4520852
C	1.6516564	-0.6879681	-3.6421682
C	0.3839568	-0.6194718	-4.2249485
H	-1.7071835	-0.1677558	-3.9100267
H	2.5078655	-1.0191934	-4.2488771
H	0.2438569	-0.8905161	-5.2826482
C	-1.8248646	0.5754456	-1.3408366
H	-1.5156968	0.9137973	-0.3311457
C	-2.5429936	1.7534587	-2.0359007
H	-3.3734719	2.1257764	-1.4012161
H	-1.8647325	2.6038542	-2.2489345
H	-2.9891786	1.4404393	-3.0020643
C	-2.8070029	-0.5991096	-1.1456077
H	-3.6930724	-0.2661793	-0.5653754
H	-3.1720746	-0.9795911	-2.1224981
H	-2.3201040	-1.4351553	-0.6050384
C	3.2875821	-0.4776273	-1.7419170
H	3.2532714	-0.2730702	-0.6533628
C	4.2366254	0.5399253	-2.4112860
H	3.8578833	1.5804123	-2.3437109
H	5.2388862	0.5089514	-1.9361762
H	4.3737007	0.3149686	-3.4895653
C	3.8392393	-1.9096427	-1.9027659
H	4.8418161	-1.9854677	-1.4339595
H	3.1821552	-2.6510949	-1.4090966
H	3.9492199	-2.1907237	-2.9709883
C	0.8786684	-1.8510201	0.8637746
S	-0.3775617	-2.8739111	0.4728522
S	2.4897357	-2.1284742	1.3405273

$IDipp\text{-}CS_2$

Energy = -1993.590615953

S	-0.0006451	1.5410945	2.5892932
S	0.0014418	-1.5452959	2.5870133
C	0.0003067	-0.0016814	1.9047064
C	0.0000568	-0.0008679	0.4181877
N	-1.0994346	-0.0006726	-0.3986035
N	1.0992531	-0.0007236	-0.3990456
C	-0.6844603	-0.0005922	-1.7303844
C	-2.4896623	-0.0000796	0.0191588
C	0.6837734	-0.0004651	-1.7306670
C	2.4894724	-0.0003098	0.0187043
H	-1.4055106	-0.0007642	-2.5515025
C	-3.1450376	-1.2475421	0.1903130
C	-3.1441616	1.2480850	0.1889175
H	1.4044708	-0.0001165	-2.5521026
C	3.1437538	1.2477792	0.1897627
C	3.1449886	-1.2478511	0.1888722
C	-4.5092191	-1.2131647	0.5424821
C	-2.4433918	-2.5848677	-0.0433378
C	-4.5084048	1.2150947	0.5409877
C	-2.4412796	2.5847110	-0.0452592
C	4.5077944	1.2146549	0.5426249
C	2.4410776	2.5844981	-0.0444495
C	4.5089944	-1.2136069	0.5417070
C	2.4436510	-2.5850897	-0.0462308
C	-5.1844905	0.0012942	0.7160668
H	-5.0502893	-2.1598942	0.6867890
H	-1.3505709	-2.4010270	0.0099427
H	-5.0487593	2.1623854	0.6843766
H	-1.3486148	2.3998944	0.0086308
C	5.1839600	0.0007910	0.7169221
H	5.0479670	2.1618856	0.6871024
H	1.3483515	2.3996927	0.0081984
H	5.0501359	-2.1603841	0.6854155
H	1.3507823	-2.4014405	0.0065736
H	-6.2496469	0.0018338	0.9944769
H	6.2489620	0.0012307	0.9959165
C	2.7784272	-3.1374024	-1.4492141
H	2.4984448	-2.4273260	-2.2537261
H	3.8650310	-3.3420745	-1.5499246
H	2.2370952	-4.0882388	-1.6341764
C	2.7574927	-3.6207472	1.0483042
H	2.1514064	-4.5356485	0.8885850
H	3.8235728	-3.9297312	1.0426574
H	2.5085888	-3.2210765	2.0507579
C	-2.7774129	-3.1385196	-1.4459381
H	-2.2358280	-4.0894384	-1.6297132
H	-3.8639320	-3.3434611	-1.5470366
H	-2.4970810	-2.4291519	-2.2509547
C	-2.7575802	-3.6195543	1.0520371
H	-2.5093428	-3.2188934	2.0542646
H	-3.8235698	-3.9288608	1.0461188
H	-2.1511169	-4.5344192	0.8935608
C	-2.7550741	3.6202797	1.0494659
H	-3.8206500	3.9310462	1.0423424
H	-2.5083817	3.2196194	2.0521266
H	-2.1471806	4.5342818	0.8912255
C	-2.7739828	3.1380954	-1.4482912
H	-2.2314710	4.0885119	-1.6320508
H	-2.4937303	2.4282144	-2.2528861
H	-3.8602757	3.3439288	-1.5501316
C	2.7538357	3.6197505	1.0508454
H	3.8195481	3.9300738	1.0451681
H	2.1465408	4.5340339	0.8919299
H	2.5056332	3.2189960	2.0530983
C	2.7751697	3.1381745	-1.4470663
H	2.2327876	4.0885819	-1.6312607

H	3.8615587	3.3440937	-1.5477049
H	2.4958630	2.4283730	-2.2520722

IMes-CS_2

Energy = -1757.905078918

S	-1.4432273	2.6486769	0.1272033
S	-1.6160960	0.2574238	2.0512252
C	-1.9943791	1.8027433	1.4820757
C	-2.9808396	2.5459944	2.3168021
N	-2.6997543	3.3752533	3.3687928
N	-4.3426509	2.5313784	2.1799569
C	-3.8903950	3.8802271	3.8910236
C	-1.3874149	3.7031144	3.8879622
C	-4.9140268	3.3545434	3.1502029
C	-5.1083210	1.7926326	1.1964193
H	-3.8911681	4.5669270	4.7418947
C	-0.8523624	2.9084530	4.9287482
C	-0.7194426	4.8394846	3.3734898
H	-5.9974924	3.4852029	3.2174701
C	-5.4199414	2.4208490	-0.0309151
C	-5.5590289	0.4912492	1.5256525
C	0.4114707	3.2696215	5.4331437
C	-1.5987252	1.7152370	5.4703285
C	0.5404880	5.1501290	3.9183322
C	-1.3261553	5.6785858	2.2772152
C	-6.1882790	1.6868344	-0.9561132
C	-4.9385835	3.8146250	-0.3467634
C	-6.3223039	-0.1910534	0.5614313
C	-5.2214163	-0.1444862	2.8507752
C	1.1272777	4.3770326	4.9391627
H	0.8483543	2.6590598	6.2397755
H	-1.0383300	1.2398745	6.2973868
H	-2.6031109	1.9933806	5.8538251
H	-1.7505771	0.9601102	4.6658348
H	1.0794710	6.0275789	3.5260079
H	-0.6746345	6.5378659	2.0296590
H	-1.4673043	5.0651835	1.3584503
H	-2.3226826	6.0767895	2.5628850
C	-6.6437782	0.3835734	-0.6849762
H	-6.4319479	2.1543279	-1.9236413
H	-3.8253018	3.8458181	-0.3477206
H	-5.2998446	4.1423933	-1.3398119
H	-5.2881604	4.5538793	0.4046111
H	-6.6725791	-1.2095590	0.7949285
H	-4.1178613	-0.2529463	2.9544746
H	-5.5733266	0.4696327	3.7065055
H	-5.6829556	-1.1462146	2.9383871
C	2.5015479	4.7124249	5.4701433
C	-7.4644821	-0.3855343	-1.6943028
H	2.6926108	5.8038976	5.4530746
H	2.6398564	4.3521475	6.5086378
H	3.2904952	4.2344060	4.8498713
H	-7.0041764	-1.3698158	-1.9197908
H	-8.4863851	-0.5899863	-1.3101981
H	-7.5668301	0.1682341	-2.6474322

[cAAC^{Me}-CS_2]$^{-}$

Energy = -1669.320988381

C	0.7199019	-0.4261163	0.9920678
C	0.9057041	0.3851259	2.2927683
C	0.5387656	1.8196245	1.8366323
C	0.7917098	1.8953683	0.3183452
H	-0.5421904	1.9969574	2.0214973
H	1.0999976	2.6014133	2.3896892
C	-0.0642665	-0.0804634	3.4026307
H	-1.1162786	-0.0444150	3.0507461
H	0.1754535	-1.1262946	3.6833925
H	0.0296860	0.5773825	4.2951471
C	2.3504341	0.3204011	2.8547217
H	2.5768484	-0.7363044	3.1052585
H	3.1052765	0.6681979	2.1214175
H	2.4357094	0.9612571	3.7614546
C	-0.1658093	2.9035633	-0.3381767
H	0.0729189	3.9211462	0.0359548
H	-0.0570266	2.9132418	-1.4407637
H	-1.2217057	2.6910398	-0.0881237
C	2.2308148	2.3509620	-0.0199177
H	2.3887047	2.3565643	-1.1167655
H	2.3990432	3.3823438	0.3554266
H	2.9935117	1.6941109	0.4354171
N	0.5417928	0.4658317	-0.0869438
C	0.5940470	0.1297885	-1.4946957
C	-0.5632812	0.3680406	-2.3097545
C	1.8336476	-0.2394667	-2.1159642
C	-0.4403447	0.2875112	-3.7090705
C	1.8909937	-0.3091210	-3.5219771
C	0.7774347	-0.0326805	-4.3242485
H	-1.3318298	0.4576498	-4.3341182
H	2.8402085	-0.6002350	-4.0002563
H	0.8527133	-0.0847618	-5.4224433
C	-1.9643300	0.5637126	-1.7190166
H	-1.8331159	0.7479200	-0.6339085
C	-2.7374985	1.7469867	-2.3348368
H	-3.7007863	1.8984560	-1.8022673
H	-2.1716214	2.6992924	-2.2944130
H	-2.9886804	1.5563850	-3.4001079
C	-2.7943944	-0.7321096	-1.8493958
H	-3.7851150	-0.6097064	-1.3595994
H	-2.9711772	-0.9866210	-2.9169457
H	-2.2499252	-1.5704254	-1.3647919
C	3.0742464	-0.6757042	-1.3295943
H	2.8869821	-0.4729655	-0.2568839
C	4.3559779	0.0753086	-1.7464707
H	4.2479605	1.1761871	-1.6735045
H	5.2061107	-0.2273764	-1.0989587
H	4.6464922	-0.1620114	-2.7922933
C	3.2922698	-2.2012647	-1.4559542
H	4.1150281	-2.5294494	-0.7867203
H	2.3706621	-2.7519510	-1.1753233
H	3.5653116	-2.4760336	-2.4986430
C	0.6508766	-1.8621830	0.8986909
S	-0.1271108	-2.6045090	-0.4605471
S	1.4044523	-2.8196008	2.1397372

[IDipp-CS_2]$^{-}$

Energy = -1993.621502782

S	1.5395127	0.0006825	2.7636872
S	-1.5402610	-0.0013553	2.7633121
C	-0.0002672	-0.0003078	1.9517386
C	-0.0000923	-0.0002653	0.5314765
N	-1.1187925	-0.0005964	-0.3384240
N	1.1188354	-0.0000218	-0.3381220
C	-0.6819320	-0.0005778	-1.6646519
C	-2.5355080	-0.0003125	-0.0512872
C	0.6823266	-0.0001870	-1.6644663
C	2.5354878	0.0001764	-0.0506310
H	-1.3975791	-0.0008196	-2.4914260
C	-3.2365851	-1.2411673	-0.0830805
C	-3.2359108	1.2409828	-0.0818868
H	1.3981981	-0.0000352	-2.4910501
C	3.2361147	1.2412952	-0.0823186
C	3.2363262	-1.2408593	-0.0813670
C	-4.6426424	-1.2120429	-0.0691025
C	-2.4957021	-2.5757167	-0.0382271
C	-4.6419829	1.2125992	-0.0677948
C	-2.4943461	2.5751252	-0.0359914
C	4.6421875	1.2126677	-0.0687572
C	2.4947720	2.5755750	-0.0368889
C	4.6423876	-1.2119720	-0.0676967
C	2.4952444	-2.5752563	-0.0351378
C	-5.3494258	0.0004598	-0.0582416
H	-5.1991373	-2.1635698	-0.0615075
H	-1.4139752	-2.3510874	-0.1340922
H	-5.1979590	2.1644253	-0.0590469
H	-1.4127327	2.3500432	-0.1320616
C	5.3494023	0.0004158	-0.0582757
H	5.1983441	2.1643904	-0.0611548
H	1.4130904	2.3506011	-0.1324799
H	5.1987048	-2.1635949	-0.0591664
H	1.4135208	-2.3505540	-0.1308600
H	-6.4511698	0.0007529	-0.0498071
H	6.4511455	0.0005137	-0.0500647
C	2.8797615	-3.5044271	-1.2027083
H	2.6964750	-3.0235304	-2.1860581

H	3.9529892	-3.7897623	-1.1650859
H	2.2885504	-4.4442051	-1.1670875
C	2.6912162	-3.2588998	1.3343543
H	2.0757179	-4.1812187	1.4052268
H	3.7533813	-3.5463999	1.4923333
H	2.3871012	-2.5622089	2.1445633
C	-2.8807030	-3.5038230	-1.2064825
H	-2.2895488	-4.4436758	-1.1719256
H	-3.9539348	-3.7891230	-1.1687335
H	-2.6977422	-3.0220502	-2.1894630
C	-2.6913659	-3.2604958	1.3307402
H	-2.3869452	-2.5645454	2.1414758
H	-3.7535358	-3.5479453	1.4887788
H	-2.0760051	-4.1829833	1.4006376
C	-2.6896175	3.2589687	1.3335111
H	-3.7516124	3.5469506	1.4917754
H	-2.3855810	2.5622159	2.1437001
H	-2.0736948	4.1810261	1.4041262
C	-2.8789313	3.5043172	-1.2035192
H	-2.2872860	4.4438353	-1.1682652
H	-2.6962627	3.0232093	-2.1868815
H	-3.9520181	3.7901336	-1.1654922
C	2.6906361	3.2600041	1.3322225
H	3.7527467	3.5478276	1.4899829
H	2.0749286	4.1822206	1.4026237
H	2.3867639	2.5636762	2.1428392
C	2.8790868	3.5041809	-1.2049767
H	2.2876580	4.4438424	-1.1698998
H	3.9522444	3.7897999	-1.1675066
H	2.6959278	3.0226787	-2.1880538

[IMes-CS_2]$^-$

Energy = -1757.924967338

S	-2.3492652	0.7424527	-0.1263543
S	-0.0441697	1.9388757	1.5302574
C	-1.7245800	1.7293631	1.1556587
C	-2.6660121	2.4707616	1.9298623
N	-2.3824558	3.4433255	2.9182674
N	-4.0599125	2.5768907	1.7085721
C	-3.5455196	4.1629154	3.2026621
C	-1.1791456	3.6805607	3.6714457
C	-4.5666185	3.6355755	2.4659074
C	-4.9485845	1.7377186	0.9485407
H	-3.5431059	4.9627125	3.9490586
C	-0.8522585	2.8296254	4.7661159
C	-0.5163977	4.9273640	3.5026409
H	-5.6315004	3.8848173	2.4411894
C	-5.6055985	2.3025503	-0.1784130
C	-5.3834540	0.4946096	1.4923740
C	0.1571941	3.2356589	5.6511775
C	-1.5263649	1.4920381	4.9047497
C	0.4822455	5.2892982	4.4244894
C	-0.7800154	5.7528718	2.2693235
C	-6.6784474	1.5984274	-0.7551266
C	-5.0462126	3.5437823	-0.8248823
C	-6.4530804	-0.1684925	0.8742926
C	-4.6418384	-0.1187177	2.6484140
C	0.8392901	4.4647438	5.5091816
H	0.4200304	2.5660940	6.4887387
H	-1.2227856	0.9772945	5.8380151
H	-2.6330138	1.5791492	4.8934399
H	-1.2425077	0.8625573	4.0314914
H	1.0146408	6.2448563	4.2749159
H	-0.1549375	6.6681755	2.2539470
H	-0.5330714	5.1307248	1.3789096
H	-1.8430267	6.0558478	2.1620211
C	-7.1269348	0.3638665	-0.2483252
H	-7.1675008	2.0239289	-1.6488359
H	-3.9981280	3.3288356	-1.1351262
H	-5.6340357	3.8345045	-1.7185949
H	-5.0032103	4.4154547	-0.1381779
H	-6.7747962	-1.1409791	1.2862761
H	-3.6084216	-0.3618841	2.3131162
H	-4.5466251	0.5835159	3.5028192
H	-5.1362777	-1.0439960	3.0053965
C	1.9392979	4.8576577	6.4699470
C	-8.2877593	-0.3749179	-0.8761164
H	2.1551269	5.9447990	6.4228616
H	1.6780967	4.6101465	7.5211366
H	2.8923903	4.3266901	6.2466089
H	-8.0057677	-1.4076485	-1.1769444
H	-9.1472126	-0.4741778	-0.1755420
H	-8.6585627	0.1455765	-1.7823823

[K(18-crown-6)(cAAC^{Me}-CS_2)]

Energy = -3193.292315235

S	4.1826639	6.0484695	14.2036377
C	4.6308744	6.9600828	15.6202477
S	3.5661154	8.2117466	16.2274251
C	5.8733920	6.6972374	16.2994708
N	6.7896794	5.6997897	15.9535049
C	7.8133811	5.4716528	17.0499243
C	7.8004691	6.8417480	17.7521349
H	8.5482114	7.4996077	17.2612520
H	8.0851245	6.7660879	18.8208632
C	6.3839718	7.4438379	17.5617639
C	6.5285282	8.9718057	17.3499988
H	7.1440911	9.1962545	16.4545373
H	7.0388617	9.4151255	18.2325816
H	5.5371558	9.4440640	17.2173073
C	5.4822084	7.2011980	18.7983458
H	4.4720788	7.6101371	18.6007619
H	5.9142751	7.7107864	19.6858570
H	5.3790218	6.1251831	19.0397085
C	9.2063121	5.1340529	16.4994284
H	9.2187004	4.1658859	15.9620711
H	9.9180964	5.0657264	17.3473719
H	9.5745761	5.9131754	15.8054398
C	7.3781843	4.3505898	18.0231862
H	6.3302445	4.4780944	18.3543001
H	8.0255410	4.3743571	18.9240282
H	7.4797034	3.3486260	17.5697163
C	7.0265338	5.1415106	14.6371062
C	6.7747363	3.7608067	14.3745148
C	7.1872359	3.2199182	13.1415694
H	6.9883417	2.1569453	12.9319123
C	7.8204802	4.0031337	12.1695769
H	8.1352848	3.5582143	11.2126246
C	8.0424130	5.3604715	12.4270925
H	8.5288335	5.9828593	11.6594253
C	7.6669251	5.9531614	13.6481264
C	5.9863918	2.8586017	15.3246385
H	5.7622002	3.4552415	16.2293868
C	4.6274410	2.4574830	14.7129919
H	4.0559968	3.3684288	14.4435391
H	4.0343089	1.8644369	15.4413635
H	4.7589957	1.8361992	13.8017902
C	6.7783891	1.6025479	15.7414863
H	6.9433235	0.9239182	14.8783997
H	6.2241706	1.0246219	16.5106751
H	7.7781655	1.8492136	16.1540279
C	7.9090968	7.4528093	13.8242366
H	7.6683866	7.7105693	14.8735865
C	6.9510843	8.2681755	12.9276988
H	7.1952526	8.1216835	11.8534333
H	7.0358702	9.3530928	13.1489368
H	5.9015059	7.9490148	13.0884754
C	9.3744187	7.8624001	13.5735314
H	9.6772327	7.6910966	12.5193793
H	10.0815154	7.2985636	14.2160562
H	9.5157216	8.9435497	13.7820194
K	1.5797309	7.9014520	13.7825300
O	-0.3215742	8.6937658	16.0222870
C	0.2048695	9.9076393	16.5359007
H	1.2789567	9.7860104	16.8141909
H	-0.3545710	10.2243210	17.4520510
C	0.0669184	10.9942627	15.4880235
H	-0.9959086	11.0584872	15.1470698
H	0.3328557	11.9766575	15.9510733
O	0.9253555	10.7119981	14.3939380
C	0.8962791	11.6957883	13.3791448
H	1.1433690	12.7048997	13.7939757
H	-0.1198608	11.7635060	12.9169454
C	1.9194067	11.3481072	12.3150393

H	1.9732955	12.1885292	11.5789797
H	2.9277990	11.2444471	12.7848358
O	1.5353789	10.1424592	11.6733808
C	2.4104096	9.7559025	10.6260124
H	3.4434514	9.5830779	11.0144500
H	2.4720689	10.5548164	9.8455958
C	1.8887269	8.4851047	9.9835665
H	0.8425600	8.6471645	9.6231859
H	2.5192150	8.2530663	9.0893205
O	1.9394709	7.4305726	10.9245669
C	1.5456996	6.1739084	10.3948022
H	2.2046719	5.8863109	9.5387070
H	0.4960193	6.2211702	10.0130344
C	1.6531388	5.1125721	11.4714266
H	1.4930326	4.1106420	11.0001661
H	2.6788637	5.1260525	11.9116843
O	0.6735478	5.3580881	12.4705044
C	0.7188641	4.4079528	13.5292908
H	1.7298844	4.4083070	14.0039176
H	0.5075379	3.3798274	13.1427106
C	-0.3238703	4.7654346	14.5700818
H	-1.3346857	4.8414409	14.0971409
H	-0.3661751	3.9427619	15.3259846
O	0.0394252	5.9891320	15.1830102
C	-0.7589222	6.3545786	16.2940215
H	-0.7683556	5.5382491	17.0579956
H	-1.8171139	6.5363313	15.9807947
C	-0.1808533	7.6046445	16.9279532
H	-0.7304421	7.8126315	17.8799535
H	0.8983179	7.4415408	17.1682974

[K(18-crown-6)(IDipp-CS_2)]

Energy = -3517.829972356

O	-0.8730397	7.7986538	10.7909512
C	-1.0784609	7.0235612	9.6145824
H	-2.1666060	6.8033859	9.4761600
H	-0.5274421	6.0543919	9.6927580
C	-0.5828488	7.8028152	8.4124975
H	-0.8780008	7.2549703	7.4837323
H	-1.0700755	8.8090974	8.3810108
O	0.8257750	7.9300144	8.4901095
C	1.4159328	8.5799306	7.3776445
H	1.0680109	9.6409078	7.3102699
H	1.1285727	8.0688665	6.4259237
C	2.9248722	8.5311153	7.5138374
H	3.2572835	7.4742172	7.6585105
H	3.3830283	8.9229021	6.5712966
O	3.3226168	9.3251287	8.6270637
C	4.7244999	9.2921648	8.8448948
H	5.2713953	9.7054859	7.9602575
H	5.0737498	8.2442393	9.0052980
C	5.0646075	10.1370672	10.0562316
H	6.1761190	10.2380681	10.1237872
H	4.6392028	11.1636909	9.9332663
O	4.5497222	9.5227884	11.2274398
C	4.8470139	10.2302087	12.4148970
H	4.3934336	11.2521893	12.3941017
H	5.9516932	10.3564595	12.5388227
C	4.3109100	9.4599822	13.6060950
H	4.7328397	8.4254828	13.6056007
H	4.6529376	9.9639986	14.5442819
O	2.8944919	9.4278901	13.5403928
C	2.2906470	8.7702137	14.6428449
H	2.5777256	9.2641797	15.6045287
H	2.6191648	7.7039498	14.6983008
C	0.7827722	8.8298801	14.4926011
H	0.3153895	8.4157424	15.4207196
H	0.4552679	9.8952089	14.3991477
O	0.3985560	8.0817860	13.3566276
C	-1.0059027	7.9998173	13.1731448
H	-1.4434660	9.0186085	13.0289103
H	-1.4925038	7.5471138	14.0722434
C	-1.3091697	7.1336503	11.9669576
H	-0.7974427	6.1476326	12.0737623
H	-2.4123098	6.9488571	11.9294185
S	1.5773475	4.6946946	11.3054794
C	3.0146619	4.3728482	10.3601240
S	4.0525898	5.6239001	9.7145393
C	3.3766734	3.0126533	10.1251911
N	2.9934001	1.8733205	10.8626643
C	3.5884767	0.7363559	10.3122342
H	3.4380878	-0.2497412	10.7595768
C	4.3294439	1.1243614	9.2357757
H	4.9196771	0.5398553	8.5250672
N	4.2171574	2.5100952	9.1105615
C	2.3009623	1.7869010	12.1266090
C	0.9978807	1.2210333	12.1438231
C	0.3915688	0.9991432	13.3949684
H	-0.6226108	0.5711522	13.4332836
C	1.0495327	1.3230789	14.5891064
C	2.3365667	1.8750018	14.5468989
H	2.8497790	2.1255022	15.4887871
C	2.9944300	2.1095668	13.3236981
C	4.3973310	2.7132737	13.3224774
H	4.7222440	2.8115627	12.2676589
C	0.2283017	0.9104339	10.8607135
H	0.9018382	1.1357861	10.0092853
C	4.7083228	3.1809101	7.9314698
C	3.8140375	3.4343824	6.8573986
C	4.3470437	3.9903505	5.6775329
H	3.6733265	4.2055982	4.8330271
C	5.7164012	4.2588330	5.5523937
C	6.5829141	3.9724458	6.6164540
H	7.6586175	4.1849074	6.5121322
C	6.1027077	3.4306356	7.8235081
C	2.3191278	3.1315954	6.9443297
H	2.1255583	2.6669969	7.9316961
C	7.0673120	3.1728110	8.9800341
H	6.4710216	2.7618776	9.8195709
K	2.1499317	7.8286624	11.0016658
H	6.1122206	4.6858323	4.6175231
H	0.5576679	1.1417172	15.5576335
C	1.4767256	4.4221980	6.8886357
H	1.5961536	4.9371277	5.9110756
H	0.3992888	4.1850716	7.0125447
H	1.7749699	5.1222370	7.6944806
C	1.8793823	2.1196784	5.8662944
H	2.0117521	2.5265420	4.8415969
H	2.4613299	1.1776361	5.9293913
H	0.8053743	1.8655972	5.9850513
C	-0.1669451	-0.5759558	10.7603879
H	0.7178806	-1.2424941	10.8215154
H	-0.8621460	-0.8716745	11.5741531
H	-0.6803185	-0.7802494	9.7976214
C	-0.9949127	1.8395790	10.7202276
H	-1.5095604	1.6644879	9.7518448
H	-1.7344383	1.6642607	11.5302052
H	-0.6664921	2.8981570	10.7647428
C	4.3884996	4.1368096	13.9173486
H	4.1387105	4.1207359	15.0000431
H	5.3864255	4.6097601	13.8069604
H	3.6390809	4.7637167	13.3923885
C	5.4152061	1.8012552	14.0370040
H	5.1670631	1.6724039	15.1117277
H	5.4508365	0.7916275	13.5790812
H	6.4348860	2.2365276	13.9820577
C	8.1407087	2.1280424	8.6141486
H	7.6885975	1.1668844	8.2934286
H	8.7902050	2.4815262	7.7857047
H	8.7978405	1.9202509	9.4843791
C	7.6974109	4.4874243	9.4829423
H	8.3458462	4.2956054	10.3637885
H	8.3267095	4.9647306	8.7019977
H	6.8968181	5.1960543	9.7780208

[K(18-crown-6)(IMes-CS_2)]

Energy = -3281.938171186

O	-0.9116644	7.8797751	10.5491520
C	-1.0273331	7.0357640	9.4079667
H	-2.1039727	6.8357850	9.1777154
H	-0.5140616	6.0609796	9.5998817
C	-0.3930879	7.7210655	8.2138906
H	-0.6152169	7.1186865	7.2983089
H	-0.8430654	8.7347342	8.0669806

O	1.0045558	7.8183181	8.4206272
C	1.7227666	8.3470994	7.3198977
H	1.3955705	9.3942589	7.1010798
H	1.5390825	7.7375220	6.4006843
C	3.2060289	8.3196219	7.6304784
H	3.5175924	7.2881131	7.9263724
H	3.7696880	8.6071825	6.7078347
O	3.4794625	9.2359597	8.6858656
C	4.8532104	9.2546355	9.0437538
H	5.4792442	9.6055840	8.1846193
H	5.1967924	8.2308128	9.3254952
C	5.0564076	10.2073560	10.2048633
H	6.1540218	10.3369313	10.3752340
H	4.6338662	11.2110057	9.9508452
O	4.4321463	9.6842198	11.3667442
C	4.6122134	10.4826747	12.5185898
H	4.1507943	11.4924394	12.3822014
H	5.6996422	10.6378265	12.7315269
C	3.9803516	9.7902461	13.7109697
H	4.4112569	8.7650173	13.8192796
H	4.2329480	10.3640165	14.6374187
O	2.5755209	9.7304277	13.5244274
C	1.8845274	9.1280499	14.6062505
H	2.0779821	9.6819917	15.5586913
H	2.2199893	8.0725922	14.7549668
C	0.3954230	9.1527323	14.3197116
H	-0.1493208	8.7899624	15.2270633
H	0.0669664	10.2048774	14.1302617
O	0.1212919	8.3296168	13.2037095
C	-1.2596705	8.2293427	12.8936390
H	-1.6805064	9.2351444	12.6457385
H	-1.8293366	7.8316397	13.7698336
C	-1.4512568	7.2880871	11.7210787
H	-0.9511205	6.3136614	11.9356085
H	-2.5467587	7.0953417	11.5968395
S	1.4173404	4.8191973	11.2658431
C	2.9987918	4.5277079	10.5784664
S	4.2400979	5.7392268	10.3411284
C	3.3190242	3.1862707	10.2152872
N	2.8484407	2.0058446	10.8122551
C	3.4218307	0.9024640	10.1734508
H	3.2162026	-0.1167365	10.5130362
C	4.2338555	1.3642469	9.1785234
H	4.8228874	0.8278672	8.4290926
N	4.1871295	2.7620380	9.1966341
C	2.2259669	1.8820583	12.1059514
C	0.8882033	1.4291688	12.1822664
C	0.3396840	1.1969115	13.4567491
H	-0.7039499	0.8475713	13.5263832
C	1.0755257	1.4146900	14.6375897
C	2.4017589	1.8736723	14.5177402
H	2.9988604	2.0444202	15.4291912
C	3.0031922	2.1103833	13.2675467
C	4.4277412	2.5988241	13.1696276
H	5.0324070	1.9624200	12.4899301
H	4.9161327	2.5991370	14.1635194
H	4.4720341	3.6290432	12.7556026
C	0.0566729	1.2901190	10.9330536
H	-0.0091727	2.2895230	10.4472614
H	-0.9655789	0.9349587	11.1674950
H	0.5028295	0.5938196	10.1931656
C	0.4507196	1.1949885	15.9971575
H	-0.3651200	0.4457187	15.9577735
H	0.0103261	2.1362760	16.3935700
H	1.1975111	0.8503649	16.7408518
C	4.6709180	3.5417452	8.0875874
C	3.7618212	3.9436445	7.0782912
C	4.2807804	4.6014465	5.9469677
H	3.5817422	4.9122793	5.1521829
C	5.6588483	4.8516119	5.7909020
C	6.5269807	4.4415575	6.8210753
H	7.6067349	4.6468078	6.7315118
C	6.0597670	3.7905712	7.9778697
C	2.2808781	3.6910582	7.2199933
H	1.7449910	3.9325847	6.2811692
H	1.8503440	4.3021000	8.0422823
H	2.0685089	2.6319165	7.4744447
C	6.1913453	5.5101025	4.5377493
H	6.3422162	4.7667257	3.7241880
H	7.1697319	5.9992145	4.7162380
H	5.4912653	6.2759840	4.1463455
C	6.9886063	3.4501682	9.1143673
H	6.9577578	2.3753681	9.3880093
H	6.6661710	4.0274737	10.0101511
H	8.0361356	3.7142792	8.8715137
K	2.0758409	7.9343694	11.0459242

[Mg(^{Dipp}NacNac)(cAAC^{Me}-CS_2)]

Energy = -3109.764721155

S	6.1225517	14.8814549	4.6120461
S	3.1648234	15.0930080	5.0156658
Mg	4.3667646	14.9662523	2.8102068
N	4.0796470	13.4277752	1.4368315
N	6.1053642	14.8570176	7.8469997
C	3.6855268	13.6705531	0.1725735
C	3.5034701	14.9637209	-0.3817557
H	3.1591309	14.9644159	-1.4242059
C	4.9206176	15.0285043	7.1535250
C	4.3728282	12.0804431	1.8391975
C	4.7720268	15.0100694	5.7267421
C	7.4469372	15.0583646	7.3338368
C	5.6758917	11.5432220	1.5999837
C	3.4501441	12.5031527	-0.7705257
H	2.9768928	12.8346966	-1.7125198
H	2.8163951	11.7261524	-0.3007963
H	4.4091261	12.0053565	-1.0217074
C	3.7555479	15.2215563	8.1614235
C	6.7629264	12.3353791	0.8677226
H	6.2998094	13.2733608	0.4997706
C	7.9160656	16.3994750	7.1806524
C	5.9680009	10.2448759	2.0620767
H	6.9708004	9.8245452	1.8853042
C	3.3905288	11.3052915	2.5276551
C	5.0113689	9.4770091	2.7381438
H	5.2593258	8.4628492	3.0878446
C	3.7364726	10.0097575	2.9629235
H	2.9836571	9.4029668	3.4904915
C	7.0505377	17.6352942	7.4419176
H	6.1177072	17.2957549	7.9351810
C	9.2362881	16.5936844	6.7309586
H	9.6098596	17.6202244	6.5963170
C	10.0818551	15.5140496	6.4532587
H	11.1111688	15.6917239	6.1053444
C	7.9114944	12.7333392	1.8174740
H	8.6656540	13.3511476	1.2864461
H	8.4323241	11.8373602	2.2155110
H	7.5409151	13.3138391	2.6858577
C	5.8782926	14.6649092	9.3389970
C	1.9712043	11.8201972	2.7794364
H	1.9485508	12.8851046	2.4671941
C	7.3129470	11.5797234	-0.3599992
H	6.5062310	11.2839003	-1.0613209
H	7.8512449	10.6545161	-0.0658633
H	8.0315244	12.2144531	-0.9189262
C	7.7311042	18.6459818	8.3889781
H	8.6267102	19.1055753	7.9226265
H	8.0576665	18.1796656	9.3407886
H	7.0331989	19.4728378	8.6345811
C	6.6433968	18.3285683	6.1240955
H	7.5327880	18.7326511	5.5974914
H	5.9587996	19.1783416	6.3246903
H	6.1379610	17.6280165	5.4324517
C	0.9304273	11.0631769	1.9255404
H	1.1567283	11.1221001	0.8419991
H	-0.0849876	11.4839854	2.0803131
H	0.8925335	9.9876564	2.1989504
C	1.5847929	11.7632306	4.2702978
H	0.5747523	12.1967292	4.4250864
H	2.2973752	12.3415687	4.8909705
H	1.5567946	10.7194037	4.6477647
C	6.9714581	15.3311130	10.1846909
H	7.9640021	14.8710322	10.0130985
H	6.7173370	15.2041974	11.2563074
H	7.0518476	16.4149028	9.9818022

C	2.7678592	14.0277474	8.1729538
H	2.2477076	13.9464611	7.2000695
H	2.0070969	14.1844177	8.9657628
H	3.2729579	13.0630218	8.3718805
C	4.5137160	15.3531772	9.5096729
H	4.6804035	16.4274807	9.7331584
C	8.2940417	13.9477371	7.0506746
C	7.8371005	12.4907024	7.1296920
H	6.7869007	12.4913570	7.4782057
C	9.6088042	14.2080020	6.6166968
H	10.2718897	13.3606387	6.3836595
C	8.6834517	11.6779673	8.1324606
H	9.7282886	11.5631796	7.7761995
H	8.7335159	12.1563102	9.1321294
H	8.2663993	10.6575235	8.2603967
C	7.8444824	11.8067353	5.7471309
H	8.8708508	11.7452922	5.3289752
H	7.4531846	10.7714744	5.8273190
H	7.2120381	12.3619680	5.0282962
C	5.8028345	13.1696705	9.7234763
H	6.7931362	12.6829097	9.6773517
H	5.4400167	13.0860960	10.7680415
H	5.1052798	12.6055172	9.0765280
C	2.9624227	16.5306505	7.9246880
H	2.3367633	16.4755058	7.0158845
H	2.3017912	16.7116405	8.7990075
H	3.6418009	17.4014817	7.8252068
H	3.9355757	14.9299600	10.3546556
N	4.1709092	16.4962856	1.4088795
C	3.7734880	16.2531973	0.1457349
C	4.4959406	17.8397574	1.8020487
C	5.8541794	18.2796168	1.7315768
C	3.6183247	17.4141806	-0.8212169
H	3.2845768	17.0706821	-1.8168512
H	2.8929185	18.1591768	-0.4399463
H	4.5777666	17.9574279	-0.9373301
C	6.9721260	17.3911780	1.1794799
H	6.5235919	16.4013727	0.9545282
C	6.1686634	19.5818981	2.1681610
H	7.2126698	19.9290801	2.1124686
C	3.4844915	18.7102363	2.3136315
C	5.1839972	20.4434044	2.6671721
H	5.4504557	21.4581218	3.0012291
C	3.8571879	20.0019186	2.7374577
H	3.0836453	20.6799164	3.1319418
C	8.0996648	17.1687039	2.2074746
H	8.8623702	16.4706727	1.8036463
H	8.6203263	18.1181455	2.4532138
H	7.7107248	16.7401703	3.1530431
C	2.0133244	18.2971548	2.4144095
H	1.9329999	17.2614402	2.0245573
C	7.5445520	17.9475214	-0.1421175
H	6.7579311	18.0809880	-0.9119650
H	8.0293909	18.9345059	0.0118445
H	8.3108743	17.2609082	-0.5585268
C	1.0960457	19.1949177	1.5558495
H	1.4108823	19.2242611	0.4929823
H	0.0495064	18.8266631	1.5869983
H	1.0900411	20.2411665	1.9269441
C	1.5237968	18.2823687	3.8771135
H	0.4692267	17.9393638	3.9317863
H	2.1365266	17.5996289	4.4992795
H	1.5674488	19.2959704	4.3284153

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