**Electronic Supplementary Material (ESI) for ChemComm.**


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# Stable, yet "Naked", Azo Radical Anion $ArNNAr^{\cdot-}$ and Dianion $ArNNAr^{2-}$ (Ar = 4-CN-2,6-$^{i}Pr_2$-$C_6H_2$) with Selective $CO_2$ Activation

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**Experimental Section**

All experiments were carried out under inert atmosphere by using standard Schlenk techniques and a glove box. Solvents were dried prior to use. Commercially available chemicals were bought from Energy Chemical or Alfa-Assar and used immediately. 4-Amino-3,5-diisopropylbenzonitrile was synthesized according to the reported method.[S2-3] Cyclic voltammetry was performed on a CHI660E electrochemical workstation, with platinum as the working and counter electrodes, $Ag/AgNO_3$ (0.1 M in $CH_3CN$) as the reference electrode, and 0.1 M $^nBu_4NPF_6$ as the supporting electrolyte. The EPR spectra were obtained using a Bruker EMX plus-6/1 variable-temperature X-band apparatus and simulated with the software of WINEPR SimFonia. The magnetic property was measured using a MPMS-XL7 SQUID on a sample prepared in a glove box. UV-Vis spectra were recorded on Lambda 750 spectrometer. The infrared spectra (KBr pellet) were collected on VECTOR22 FT-IR spectrometer. The NMR spectra were performed using a Bruker DRX-400 and Bruker DRX-500 (Germany) at room temperature in ppm downfield from internal $Me_4Si$. Element analyses were performed on Vario EL III elemental analyser at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences. The crystallographic data collection were carried out on a Bruker D8 Venture diffractometer with graphite-monochromated Mo K$\alpha$ radiation ($\lambda$ = 0.71073 Å) and a Bruker D8 VENTURE PHOTONII diffractometer with graphite-monochromated Ga K$\alpha$($\lambda$ = 1.34139 Å) radiation at 153(2) K using ω-scan technique. The diffraction data was integrated by using the *SAINT* program, which was also used for the intensity corrections for the Lorentz and polarization effects. Semi-empirical absorption correction was applied using the *SADABS* program. The structure was solved by direct methods and all the non-hydrogen atoms were refined anisotropically on $F^2$ by the full-matrix least-squares technique using the SHELXL-2014 or SHELXL-2018 crystallographic software package. All the hydrogen atoms were generated geometrically and refined isotropically using the riding model. The SQUEEZE option of the PLATON program[S1] was used to remove one molecule of disordered tetrahydrofuran from the formula unit of $[K_2(THF)_2(18\text{-c-}6)_2]^{2+}\cdot[\mathbf{1}\text{-}2CO_2]^{2-}$.

**Synthesis of 1**: The 4-amino-3,5-diisopropylbenzonitrile (5.06 g, 25 mmol) in $CH_2Cl_2$ (300 ml) was placed in a 500 mL round bottomed flask. The mixture of copper (II) sulfate pentahydrate (25 g) and potassium permanganate (25 g) was added and the heterogeneous mixture was refluxed for 24 h. The system was cooled to room temperature and filtered through Celite. The residue was washed by $CH_2Cl_2$ (3 x 100 mL) and $Et_2O$ (3 x 100 mL). The solvent of the filtrate was removed under vacuum, and the crude product was purified by silica gel chromatography (eluting with hexane ) to yield (2.2 g, 43.9%) of **1** as orange solid. $^1$H NMR ($CDCl_3$, 400 MHz, 298 K): δ = 1.21 (d, $^3J$(H, H) = 6.9 Hz, 24 H, -$CH_3$), 3.14 (sept, $^3J$(H, H) = 5.9 Hz, 4 H, -$CHMe_2$), 7.59 (s, 4 H, -CH arom.). $^{13}$C {$^1$H, $^{13}$C} NMR ($CDCl_3$, 100MHz, 298 K): δ = 23.89 (-$CH_3$), 27.70 (-$CHMe_2$), 112.79, 118.96, 128.20, 142.18, 151.79 (-C arom.). M.p. 173.4 $^o$C.

**Synthesis of $[Na(THF)_4]^+\bullet\mathbf{1}^{\bullet-}$:** Under argon atmosphere, compound **1** (0.12 g, 0.3 mmol) and Na (0.007 g, 0.3 mmol) were placed in a 100 ml Schlenk flask. Then THF (40 ml) was added to the mixture under stirring at room temperature. The mixture turned green after 2 days. The resultant green solution was filtered and the filtration was concentered to afford blue crystals that were suitable for X-ray crystallography. Isolated yield: 110 mg, 51.5% (crystals).

Elemental analysis calcd (%) for $C_{42}H_{64}NaN_4O_4$: C 70.85, H 9.06, N: 7.87; Found: C 70.74, H 9.15, N: 7.91. Mp 123.2 °C (decomp).

**Synthesis of $[K(THF)_4]^+\bullet\mathbf{1}^{\bullet-}$:** Under argon atmosphere, compound **1** (0.12 g, 0.3 mmol) and K (0.012 g, 0.3 mmol) were placed in a 100 ml Schlenk flask. Then THF (40 ml) was added to the mixture under stirring at room temperature. The mixture turned green after 2 hours. The resultant green solution was filtered and the filtration was concentered to afford blue crystals that were suitable for X-ray crystallography. Isolated yield: 120 mg, 54.9% (crystals). Elemental analysis calcd (%) for $C_{42}H_{64}K_4N_4O_4$: C 69.28, H 8.86, N: 7.70; Found: C 68.65, H 8.61, N: 8.00. Mp 112.5 °C (decomp).

**Synthesis of $[(18\text{-c-}6)K(THF)]_2^{2+}\bullet\mathbf{1}^{2-}$:** Under argon atmosphere, compound **1** (0.12 g, 0.3 mmol) and K (0.024 g, 0.6 mmol) were placed in a 100 ml Schlenk flask. Then THF (50 ml) was added to the mixture under stirring at room temperature. The mixture turned red after 6 hours. The resultant red solution was filtered and the filtration was concentered to afford deep red crystals that were suitable for X-ray crystallography. Isolated yield: 170 mg, 54.9% (crystals). Mp 130.4 °C (decomp).

**Synthesis of $[(15\text{-c-}5)Na(THF)]_2^{2+}\bullet\mathbf{1}^{2-}$:** Under argon atmosphere, compound **1** (0.12 g, 0.3 mmol) and Na (0.014 g, 0.6 mmol) were placed in a 100 ml Schlenk flask. Then THF (30 ml) was added to the mixture under stirring at room temperature. The mixture turned purplish red after 2 days. The resultant purplish red solution was filtered and the filtration was concentered, while the filtration did not afford crystals.

**Reaction of $[K(THF)_4]^+\bullet\mathbf{1}^{\bullet-}$ with $CO_2$:** At ambient temperature, the freshly made compound $[K(THF)_4]^+\mathbf{1}^{\bullet-}$ (0.15 g, 0.2 mmol) dissolved in 20 ml THF in 100 ml Schlenk flask. The reaction flask was attached to a Schlenk line, and pumped to vacuum, then exposed to $CO_2$ dried with $P_2O_5$ under stirring. The green solution turned red in ~2 seconds and pumped to vacuum to remove excess $CO_2$ and refilled with argon. The resultant red solution was maintained still for 12 hours to precipitate white powder. Upon filtration,the white powder was washed with 3 x 5 ml THF,3 x 5 ml methanol and 3 x 5 ml n-hexane, then dried in vacuo. Isolated yield: 10.5 mg, 63.2%. FT-IR ($cm^{-1}$): 2950 w, 2623 w, 1634 s, 1406 s, 996 s, 834 w, 703 w. $^{13}C$ NMR ($D_2O$, 100 MHz, 298 K): δ = 161.2. The filtration was concerted to afford red crystals, and characterized by X-ray crystallography and $^1H$ NMR, which were determined as compound **1**.

**Reaction of $[(18\text{-c-}6)K(THF)]_2^{2+}\bullet\mathbf{1}^{2-}$ with $CO_2$:** At ambient temperature, the freshly made compound $[(18\text{-c-}6)K(THF)]_2^{2+}\bullet\mathbf{1}^{2-}$ (0.22 g, 0.2 mmol) dissolved in 25 ml THF in 100 ml Schlenk flask. Then the flask was attached to a Schlenk line, and pumped to vacuum, then exposed to $CO_2$ dried with $P_2O_5$ under stirring. The purplish red solution turned to light green in ~3 seconds and pumped to vacuum to remove excess $CO_2$ and refilled with argon. The resultant light green solution was filtered and the filtration was concentered to afford white crystals that were suitable for X-ray crystallography. These were determined as $\{[(18\text{-c-}6)K(THF)_2][(18\text{-c-}6)K]\}^{2+}\bullet[\mathbf{1}\text{-}2CO_2]^{2-}\bullet THF$. Isolated yield: 220 mg, 83.9% (crystals). $^1H$ NMR (tetrahydrofuran-$d_8$, 500 MHz, 298 K): δ= 1.03 (d, $^3J$(H, H) = 6.4 Hz, 9 H, $-CH_3$), 1.27 (d, $^3J$(H, H) = 6.9 Hz, 15 H, $-CH_3$), 2.8 (sept, $^3J$(H, H) = 6.4 Hz, 4 H, $-CHMe_2$), 3.58 (s, 48 H, $-CH_2$ 18-crown-6.), 7.09 (s, 2 H, -CH arom.), 7.43 (s, 2 H, -CH arom.). $^{13}C$ $\{^1H, ^{13}C\}$ NMR (tetrahydrofuran-$d_8$, 125MHz, 298 K): δ= 22.57 ($-CH_3$), 26.42 ($-CHMe_2$), 71.26 ($-CH_2$ 18-crown-6.), 110.84, 118.96 (-C arom.), 120.24 (-CN), 127.50, 151.50 (-C arom.), 161.09 ($-CO_2$). FT-IR ($cm^{-1}$): 2900 m, 2225 w, 1623 m, 1466 w, 1353 w, 1285 m, 1109 s, 952 w, 838 w, 793 w, 751 w, 698 w, 613 w, 527 w. Mp 64.6 °C (decomp); Elemental analysis calcd (%) for

$C_{64}H_{104}K_2N_4O_{19}$: C 58.60, H 7.99, N: 4.27; Found: C 58.23, H 8.34, N: 4.45.

**Reaction of $\{[(18\text{-c-}6)K(THF)_2][(18\text{-c-}6)K]\}^{2+}\bullet[1\text{-}2CO_2]^{2-}$ with $NOSbF_6$:** Under argon atmosphere, compound $\{[(18\text{-c-}6)K(THF)_2][(18\text{-c-}6)K]\}^{2+}\bullet[\mathbf{1}\text{-}2CO_2]^{2-}$ (0.07 g, 0.05 mmol) and $NOSbF_6$ (0.03 g, 0.11 mmol) were placed in a 10 ml Schlenk flask. THF (3 ml) was then added to the mixture under stirring at room temperature. The mixture turned red after 1 day. The resultant red solution was filtered and the filtration was concentered to afford red powder that was determined as compound **1** by NMR. $^1$H NMR (tetrahydrofuran-$d_8$, 500 MHz, 298 K): δ = 1.21 (d, $^3J$(H, H) = 6.9 Hz, 24 H, -$CH_3$), 3.16 (sept, $^3J$(H, H) = 6.8 Hz, 4 H, -$CHMe_2$), 7.72 (s, 4 H, -CH arom.).

**Reaction of $\{[(18\text{-c-}6)K(THF)_2][(18\text{-c-}6)K]\}^{2+}\bullet[1\text{-}2CO_2]^{2-}$ with $I_2$:** Under argon atmosphere, compound $\{[(18\text{-c-}6)K(THF)_2][(18\text{-c-}6)K]\}^{2+}\bullet[\mathbf{1}\text{-}2CO_2]^{2-}$ (0.16 g, 0.12 mmol) dissolved in 0.5 ml $C_4D_8O$ (tetrahydrofuran-$d_8$) in a NMR tube. Then $I_2$ (0.30 g, 1.18 mmol) was added to the solution. And the reaction NMR tube was quickly covered with a screw cap. When shaking the NMR tube, small bubbles arise in the solution. After 10 hours, the resultant solution was characterized by NMR, which was determined to be compound **1** and 18-crown-6. A single resonance at 125.76 ppm was determined as $CO_2$ in $^{13}$C NMR spectroscopy. $^1$H NMR (tetrahydrofuran-$d_8$, 500 MHz, 298 K): δ = 1.21 (d, $^3J$(H, H) = 6.9 Hz, 24 H, -$CH_3$), 3.16 (sept, $^3J$(H, H) = 6.8 Hz, 4 H, -$CHMe_2$), 3.66 (s, 24 H, -$CH_2$ 18-crown-6.), 7.72 (s, 4 H, -CH arom.). $^{13}$C {$^1$H, $^{13}$C} NMR (tetrahydrofuran-$d_8$, 125 MHz, 298 K): δ = 24.09 (-$CH_3$), 28.67 (-$CHMe_2$), 71.34 (-$CH_2$ 18-crown-6.), 114.16 (-C arom.), 119.05 (-CN), 125.76 (-$CO_2$), 129.15, 143.02, 152.63 (-C arom.).

**Reaction of $\{[(18\text{-c-}6)K(THF)_2][(18\text{-c-}6)K]\}^{2+}\bullet[1\text{-}2CO_2]^{2-}$ with $O_2$ in solution state:** Under argon atmosphere, compound $\{[(18\text{-c-}6)K(THF)_2][(18\text{-c-}6)K]\}^{2+}\bullet[\mathbf{1}\text{-}2CO_2]^{2-}$ (0.04 g, 0.03 mmol) dissolved in ~2 ml THF in a 25 ml Schlenk flask. The flask was attached to a Schlenk line, and pumped to vacuum, then exposed to $O_2$ dried with $P_2O_5$ and the flask was closed. The colorless solution turned to red in ~30 seconds. The resultant red solution was concentrated to afford red powder, which was determined as compound **1** by NMR.

**Reaction of $\{[(18\text{-c-}6)K(THF)_2][(18\text{-c-}6)K]\}^{2+}\bullet[1\text{-}2CO_2]^{2-}$ with $O_2$ in solid state:** Under argon atmosphere, compound $\{[(18\text{-c-}6)K(THF)_2][(18\text{-c-}6)K]\}^{2+}\bullet[\mathbf{1}\text{-}2CO_2]^{2-}$ (0.04 g, 0.03 mmol) was placed in a 25 ml Schlenk flask. The flask was attached to a Schlenk line, and pumped to vacuum, then exposed to $O_2$ dried with $P_2O_5$ and kept closed. The white powder turned to red in 2 days. The resultant red solid contained compound **1**determined by NMR.

**Table S1.** Crystal data and structure refinement for **1**, $[Na(THF)_4]^+\bullet\mathbf{1}^{\bullet-}$ and $[K(THF)_4]^+\bullet\mathbf{1}^{\bullet-}$

| | **1** | $[Na(THF)_4]^+\bullet\mathbf{1}^{\bullet-}$ | $[K(THF)_4]^+\bullet\mathbf{1}^{\bullet-}$ |
|---|---|---|---|

| Formula | $C_{26}H_{32}N_4$ | $C_{42}H_{64}N_4O_4Na$ | $C_{42}H_{64}N_4O_4K$ |
|---|---|---|---|
| M/g mol$^{-1}$ | 400.56 | 711.96 | 728.07 |
| Crystal system | Orthorhombic | Monoclinic | Monoclinic |
| Space group | *P*bcn | *C*2/c | *C*2/c |
| *a*, Å | 14.844(8) | 18.399(2) | 18.731(4) |
| *b*, Å | 9.534(5) | 14.6911(16) | 15.129(3) |
| *c*, Å | 16.867(8) | 15.7048(16) | 15.467(3) |
| *α,* deg | | | |
| *β,* deg | | 103.277(3) | 104.882(4) |
| *γ,* deg | | | |
| *V*, Å$^3$ | 2387(2) | 4131.5(8) | 4236.1(16) |
| Z | 4 | 4 | 4 |
| Temperature, K | 153(2) | 153(2) | 153(2) |
| *R*1 ($I>2\sigma(I)$) | 0.0714 | 0.0666 | 0.0770 |
| *wR*2 (all data) | 0.1667 | 0.1712 | 0.1914 |

**Table S2.** Crystal data and structure refinement for $[K_2(18\text{-c-}6)_2(THF)_2]^{2+}$•**1**$^{2-*}$ and {[(18-c-

6)K(THF)$_2$][(18-c-6)K]}$^{2+}$•[**1**-2CO$_2$]$^{2-}$•THF$^*$

| | $[K_2(18\text{-c-}6)_2(THF)_2]^{2+}$•$\mathbf{1}^{2-}$ | {[(18-c-6)K(THF)$_2$][(18-c-6)K]}$^{2+}$•[**1**-2CO$_2$]$^{2-}$•THF$^*$ |
|---|---|---|
| Formula | $C_{112}H_{184}K_4N_8O_{27}$ | $C_{64}H_{104}K_2N_4O_{19}$ |
| M/g mol$^{-1}$ | 2231.06 | 1311.71 |
| Crystal system | Triclinic | Monoclinic |
| Space group | *P*-1 | *P*21/n |
| *a*, Å | 13.5116(6) | 12.9960(6) |
| *b*, Å | 14.2386(8) | 26.8623(14) |
| *c*, Å | 17.4578(8) | 22.3220(11) |
| *α,* deg | 84.410(2) | |
| *β,* deg | 68.7100(10) | 101.922(3) |
| *γ,* deg | 86.045(2) | |
| *V*, Å$^3$ | 3112.5(3) | 7624.6(7) |
| *Z* | 1 | 4 |
| Temperature, K | 153(2) | 153(2) |
| *R*1 (*I*>2σ(*I*)) | 0.0741 | 0.0725 |
| *wR*2 (all data) | 0.1917 | 0.1474 |

*There is another independent salt $[K_2(18\text{-c-}6)_2(THF)]^{2+}$•$\mathbf{1}^{2-}$, i.e. $C_{54}H_{88}K_2N_4O_{13}$, with 1:1 molar ratio to $[K_2(18\text{-c-}6)_2(THF)_2]^{2+}$•$\mathbf{1}^{2-}$, i.e. $C_{58}H_{96}K_2N_4O_{14}$, in the crystal, but its structural parameters are similar to those of $[K_2(18\text{-c-}6)_2(THF)_2]^{2+}$•$\mathbf{1}^{2-}$. The SQUEEZE option of the PLATON program[S1] was used to remove one molecule of disordered tetrahydrofuran from the formula unit of $[K_2(THF)_2(18\text{-c-}6)_2]^{2+}$·[**1**-2CO$_2$]$^{2-}$.

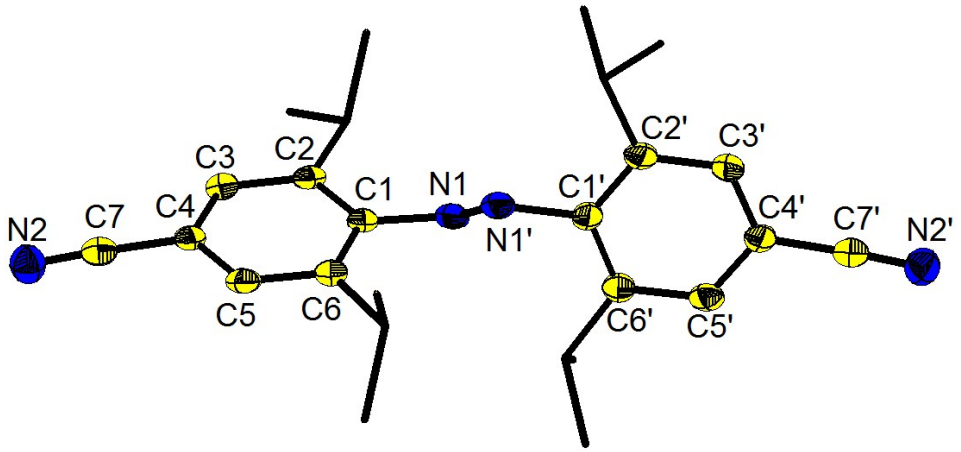



**Fig. S1.** The molecular structure of neutral azo compound **1**. The molecule lies about a twofold axis and that atoms labels with a prime character related to be unprimed atoms by the operation (1-x, -y, 1/2-z). Selected bond distances (Å) and angles (deg): N1–N1' 1.252(5), N1–C1 1.450(4), C1–C2 1.418(5), C2–C3 1.395(4), C3–C4 1.393(4), C4–C5 1.394(4), C5–C6 1.398(4), C1–C6 1.409(4), C4–C7 1.453(5), C7–N2 1.152(4), C1–N1–N1' 113.9(3), C1–N1–N1' –C1' 169.6(2).

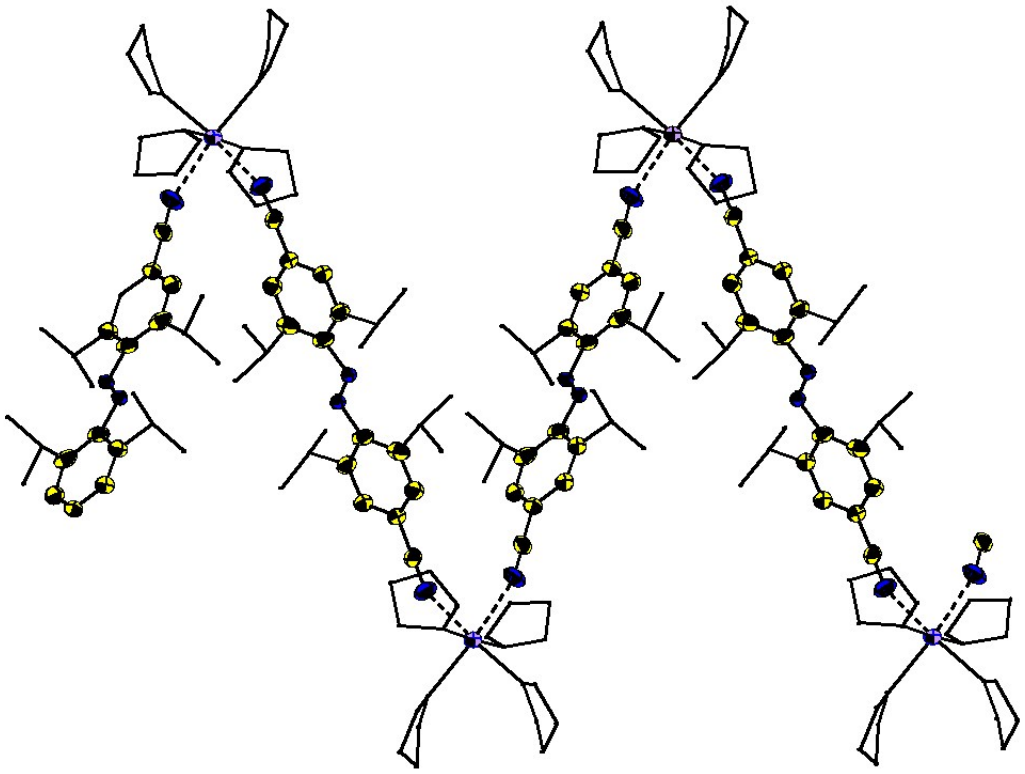


**Fig. S2**. The zig-zag geometry of the salt of $[Na(THF)_4]^{+}\cdot\mathbf{1}^{\cdot-}$.

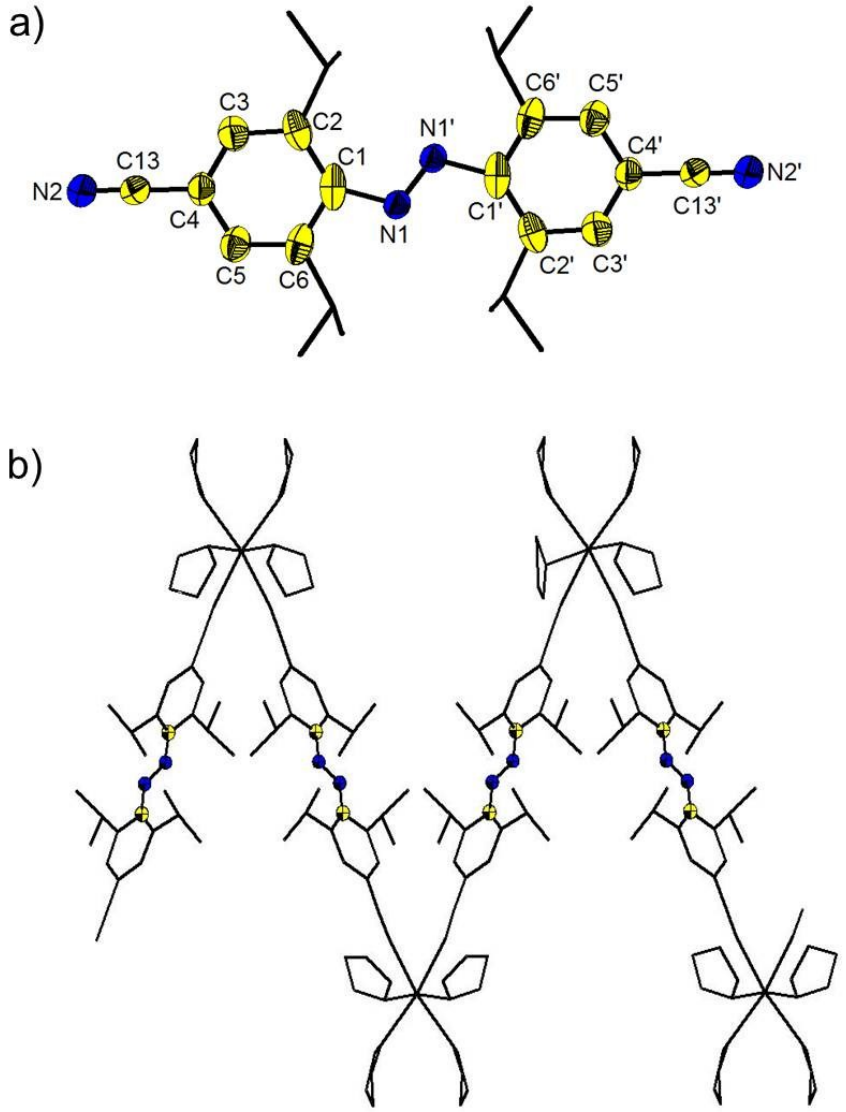



**Fig. S3.** Stick and thermal ellipsoid (50%) drawing of $[K(THF)_4]^+ \cdot \mathbf{1}^{\cdot -}$.Yellow C and blue N. Hydrogen atoms are omitted for clarity. a) The molecular geometry of $\mathbf{1}^{\cdot -}$ in $[K(THF)_4]^+ \cdot \mathbf{1}^{\cdot -}$; b) The chain geometry of the salt $[K(THF)_4]^+ \cdot \mathbf{1}^{\cdot -}$. Selected bond distances (Å) and angles (deg): N1–N1' 1.364(14), N1–C1 1.430(9), C1–C2 1.448(5), C2–C3 1.374(5), C3–C4 1.383(5), C4–C5 1.401(5), C5–C6 1.373(4), C1–C6 1.438(5), C4–C13 1.428(5), C13–N2 1.146(5), N2···K 2.805(4), C1–N1–N1' 112.2(11), C1–N1–N1' –C1' 0.0.

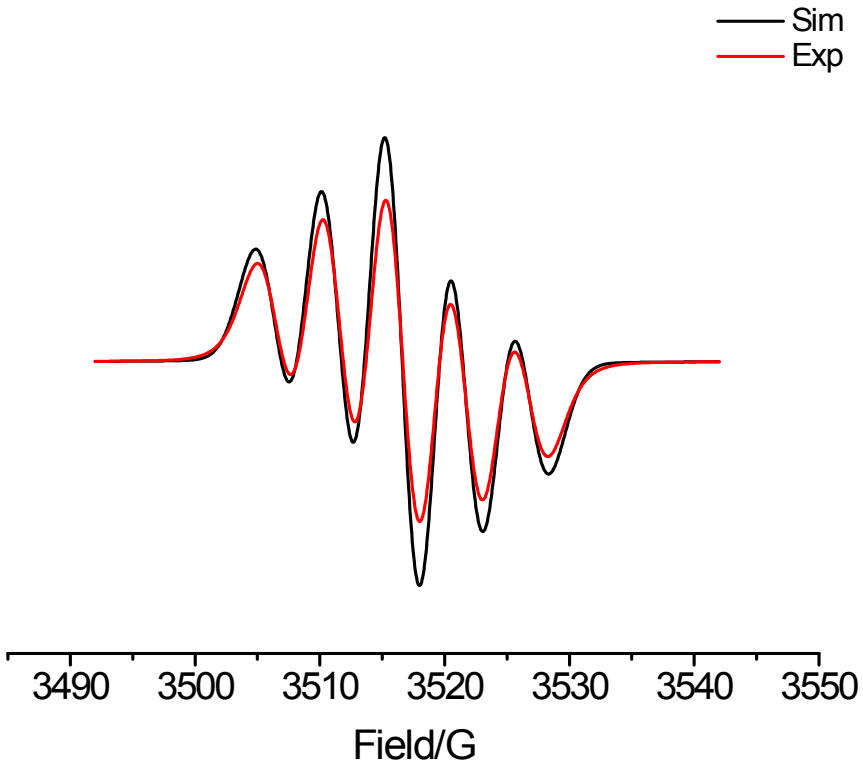



**Fig. S4**. The experimental EPR spectrum of $1\times10^{-3}$ M solution of $[K(THF)_4]^+$•**1**$^{\bullet-}$ in THF at 298 K with simulation.

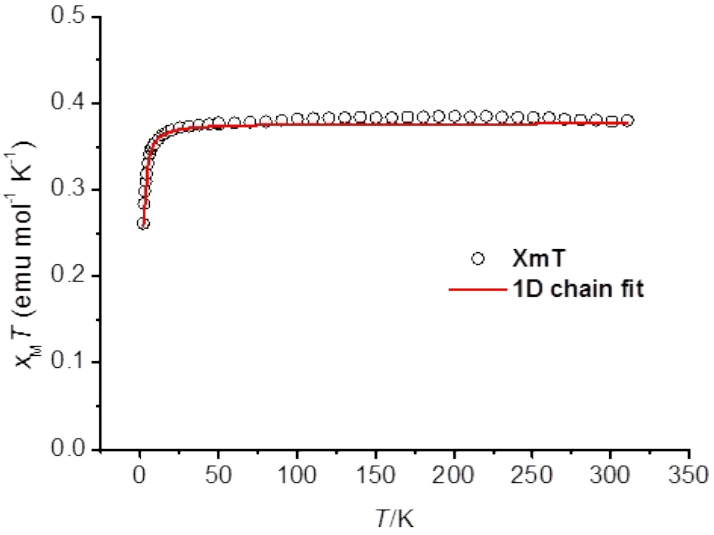



**Fig. S5**. SQUID magnetometry for polycrystalline $[Na(THF)_4]^+$•**1**$^{\bullet-}$ in the warming mode at 2000 Oe with fitting.

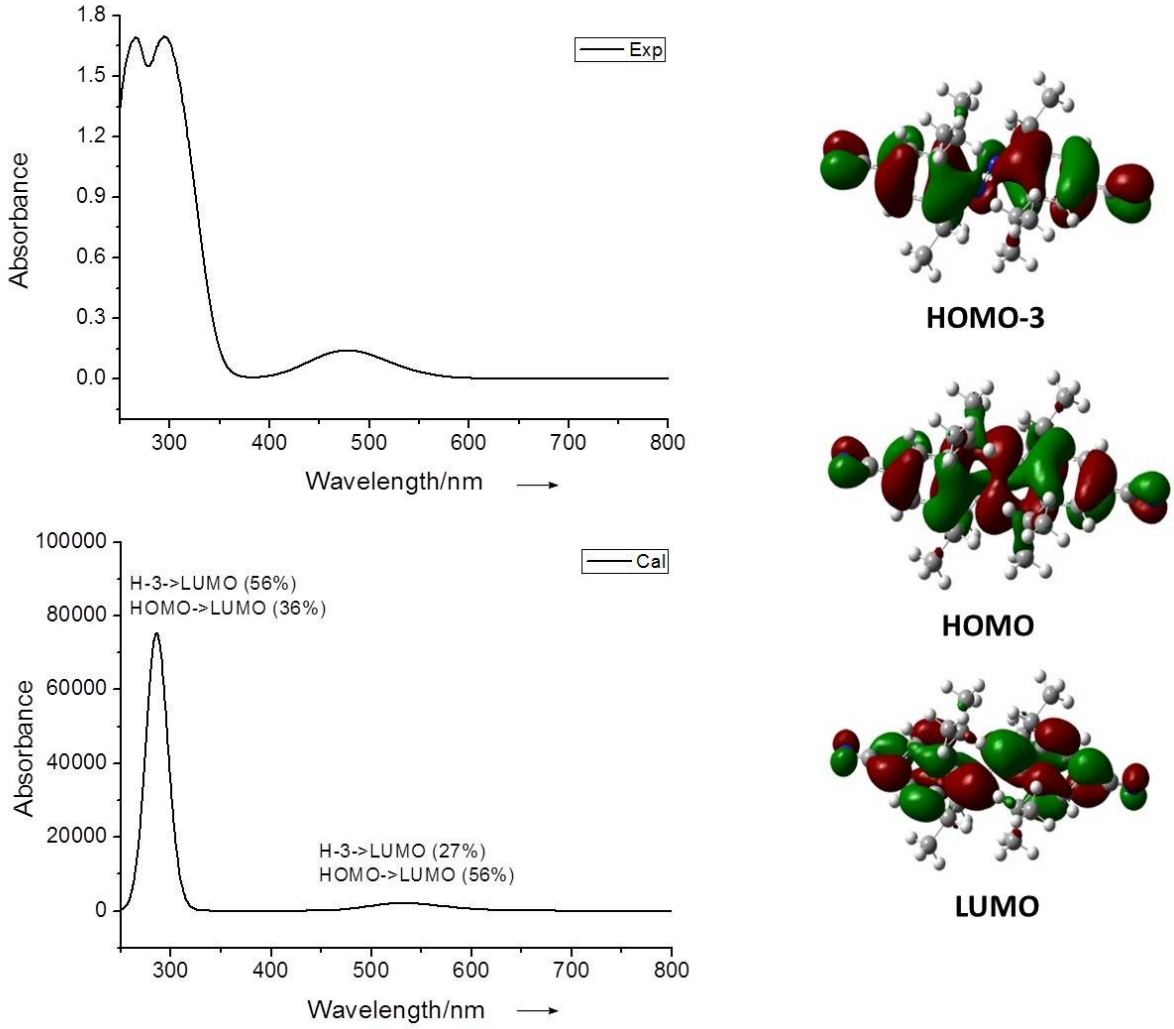



**Fig. S6.** Absorption spectrum of 1.0 x $10^{-4}$ M **1** in THF at 25 $^{o}$C (top) and calculated absorption spectrum of **1** (bottom), together with related molecular orbitals.

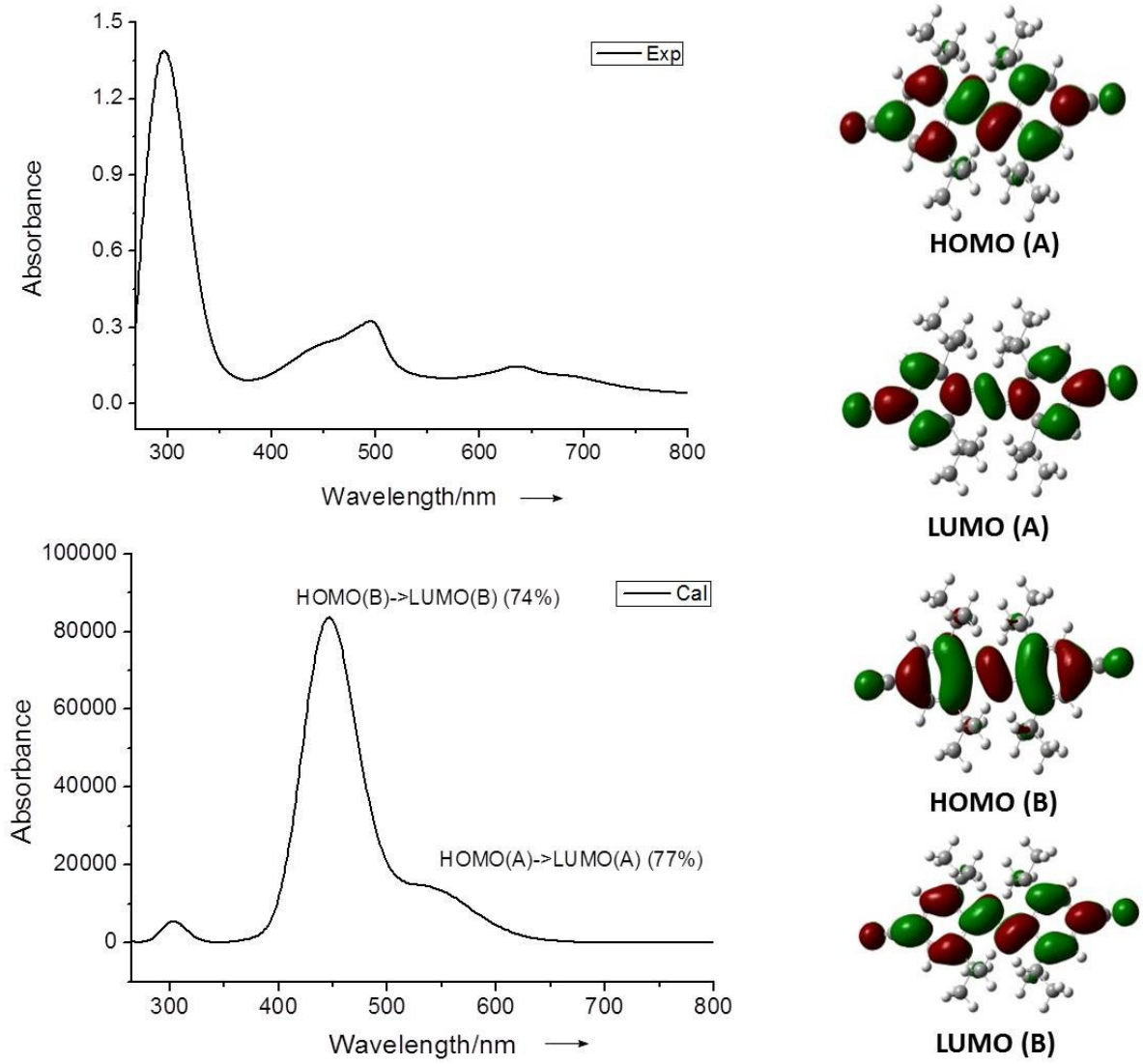



**Fig. S7.** Absorption spectrum of 1.0 x $10^{-4}$ M $[Na(THF)_4]^+$•**1**$^{\bullet-}$ in THF at 25 °C (top) and calculated absorption spectrum of the mono-radical **1**$^{\bullet-}$ (bottom), together with related molecular orbitals.

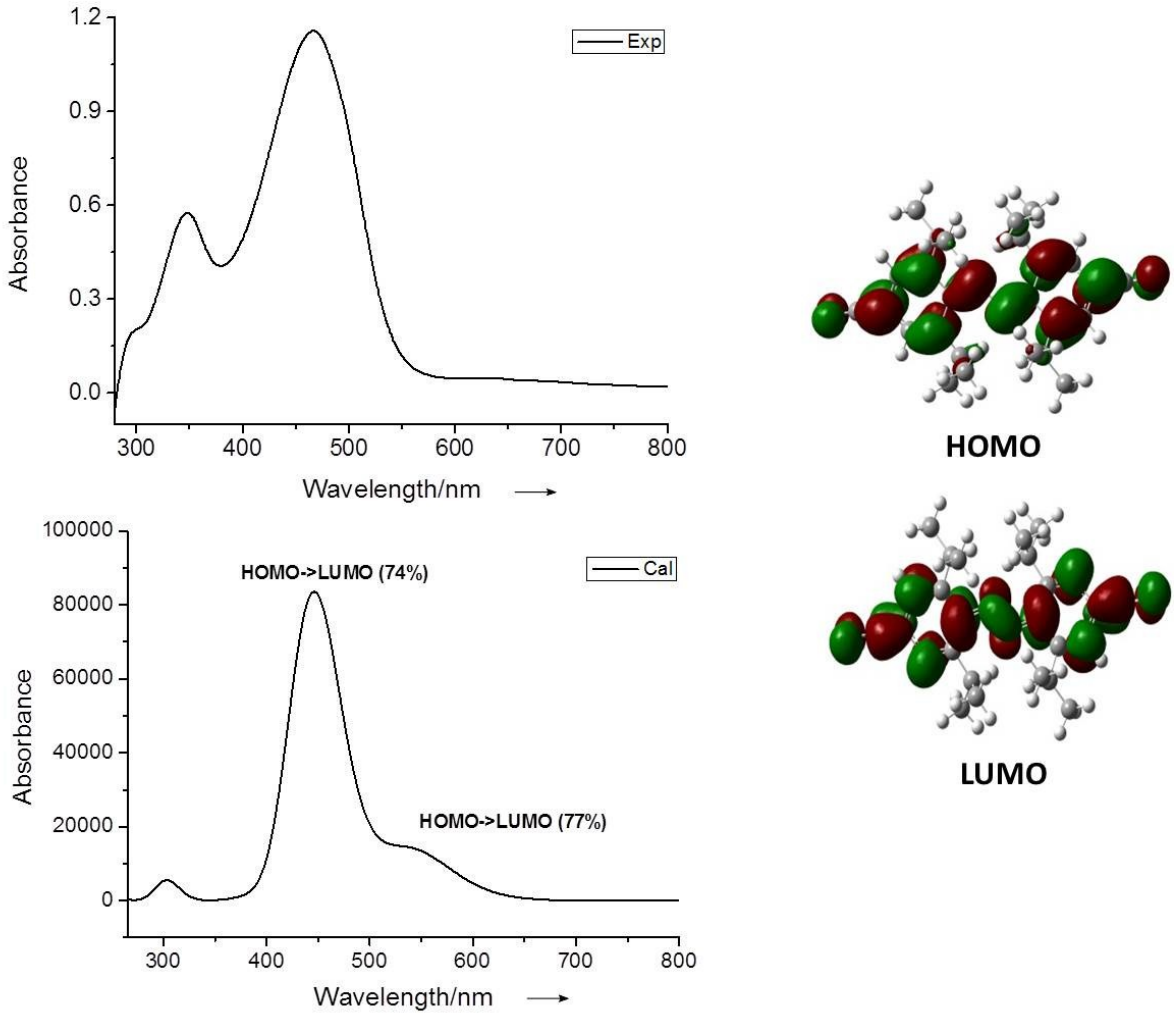



**Fig. S8.** Absorption spectrum of 1.0 x $10^{-4}$ M $[K_2(18\text{-c-}6)_2(THF)_4]^{2+}\bullet\mathbf{1}^{2-}$ in THF at 25 $^{o}$C and calculated absorption spectrum of dianion $\mathbf{1}^{2-}$, together with related molecular orbitals.

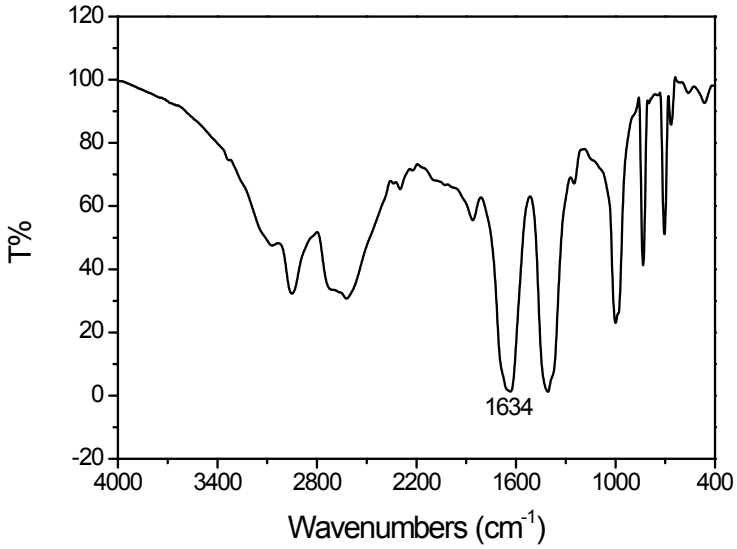



**Fig. S9.** FT-IR spectrum of the white powder from the reaction of $CO_2$ with $[(18\text{-c-}6)K(THF)]_2^{2+}\bullet\mathbf{1}^{2-}$. Peak at 1634 $cm^{-1}$ assigned to C=O in $K_2C_2O_4$.

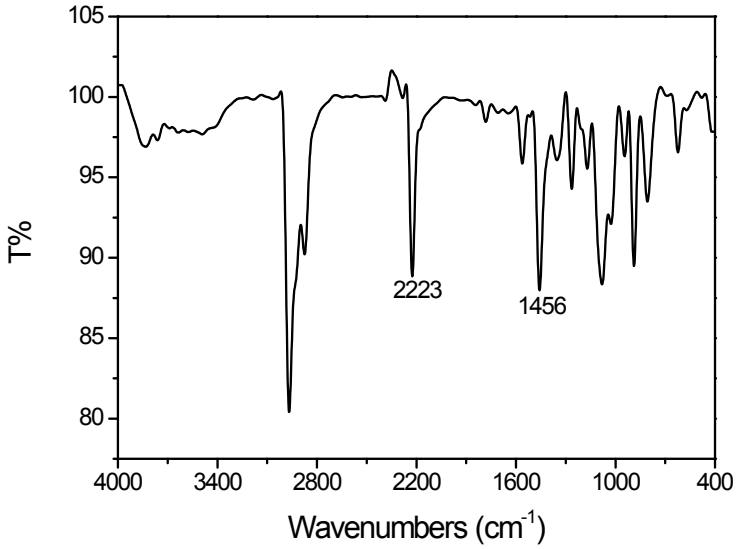



**Fig. S10.** FT-IR spectrum of compound **1**. Peak at 2223 $cm^{-1}$ assigned to C≡N, 1456 $cm^{-1}$ assigned to N=N.

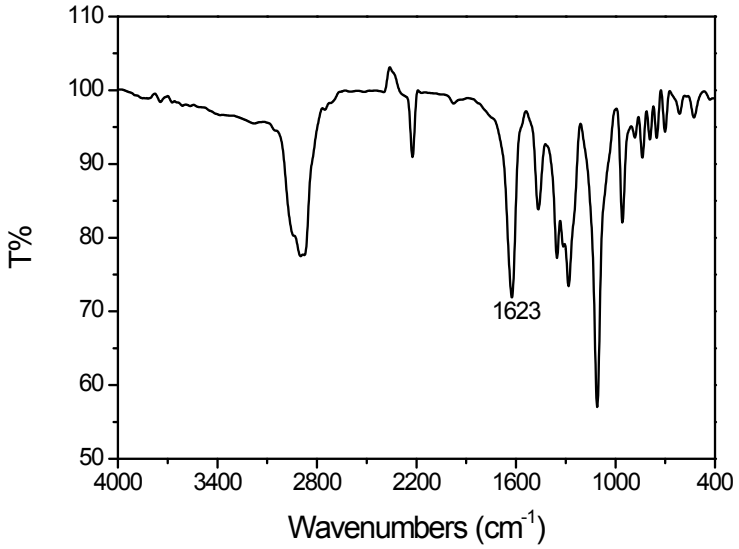



**Fig. S11** FT-IR spectrum of $\{[(18\text{-c-6})K(THF)_2][(18\text{-c-6})K]\}^{2+}\bullet[\mathbf{1}\text{-}2CO_2]^{2-}$. Peak at 1623 $cm^{-1}$ assigned to C=O.

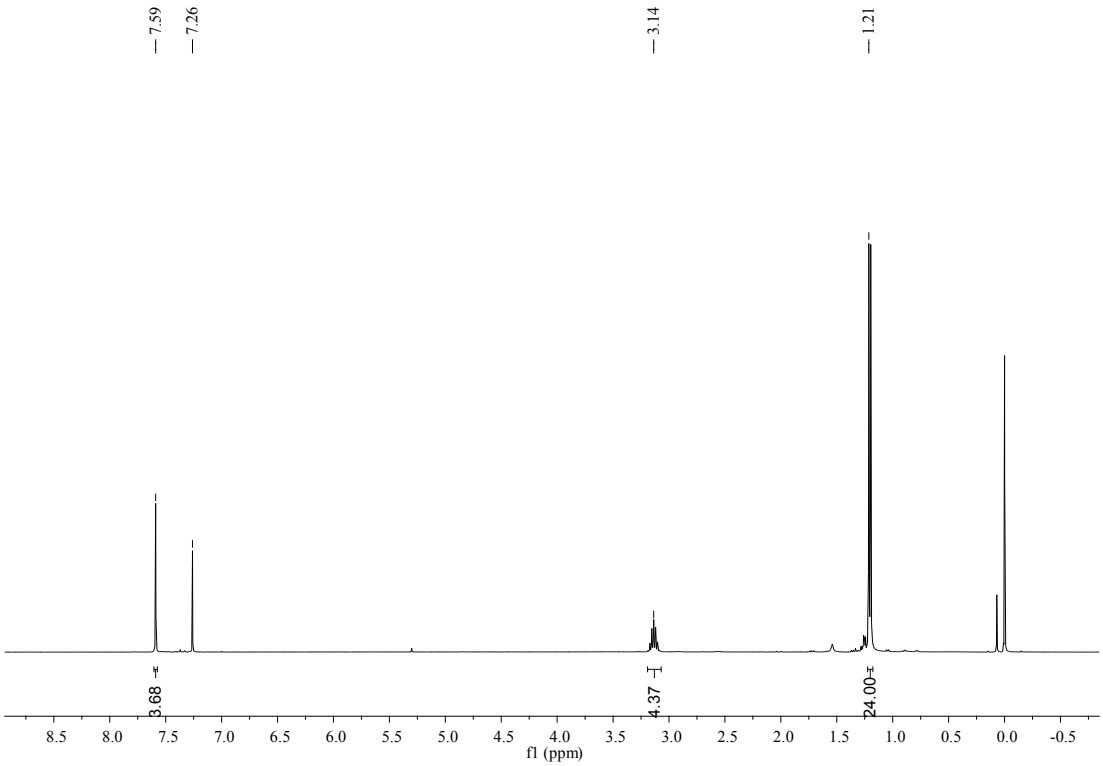



**Fig. S12.** $^{1}$H NMR spectrum of **1** from the reaction of $[K(THF)_4]^{+}$•**1**$^{\bullet-}$ with $CO_2$ ($CDCl_3$, 400MHz, 298 K).

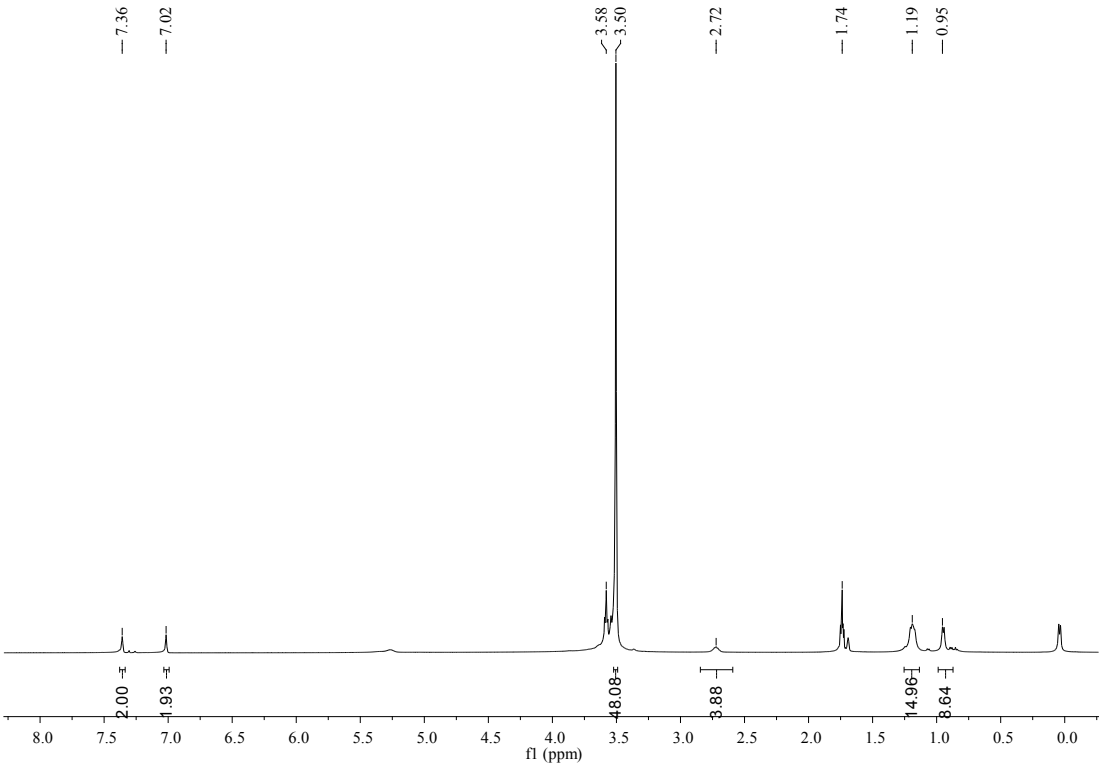


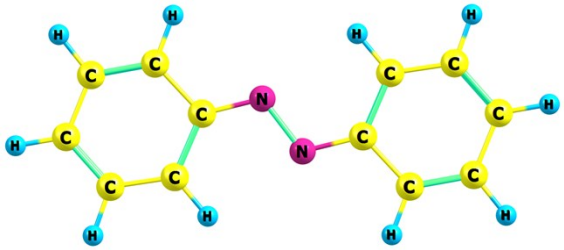

**Fig. S13.** $^{1}$H NMR spectrum of $\{[(18\text{-c-6})K(THF)_2][(18\text{-c-6})K]\}^{2+}$•[**1**-2$CO_2$]$^{2-}$ (THF-$d_8$, 500 MHz, 298 K).

**Computational details:**

All calculations were performed with the Gaussian 09 program suite.[S4] The geometry optimizations were carried out at the (U)M062x/6-31G(d) level of theory. The obtained stationary points were characterized by frequency calculations. The molecular orbitals were calculated at the level of (U)M062x/6-31G(d) on the optimized geometries. The UV-vis absorption spectra were calculated using the time-dependent DFT (TD-DFT) method at (U)M062x/6-31G(d).

**Coordinates**

**PhN=NPh**



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| C | -0.356545028 | 4.509068988 | -0.000002406 |
| C | 0.952645299 | 4.036742542 | -0.000145450 |
| H | 1.784972430 | 4.733444216 | -0.000199168 |
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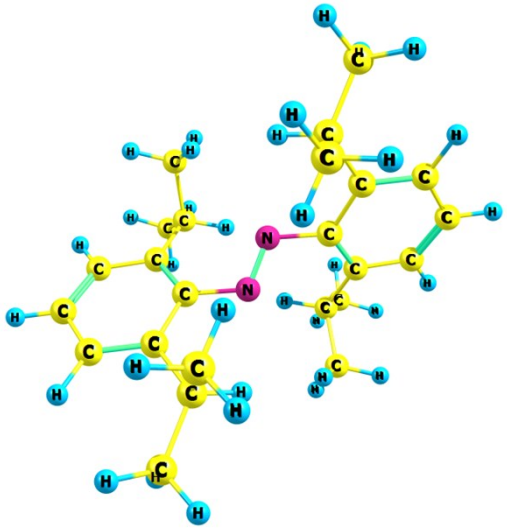
**DippN=NDipp**



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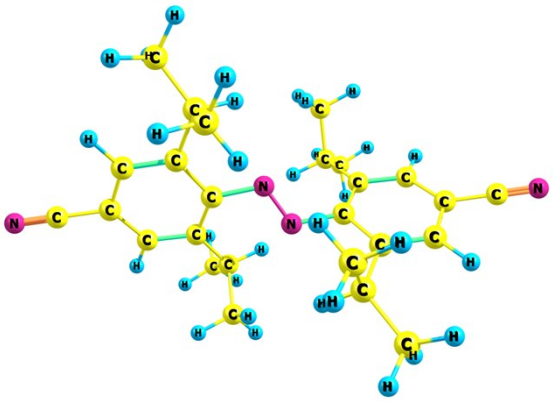
**1**



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| C | -2.029193000 | 1.746829000 | 3.225103000 |
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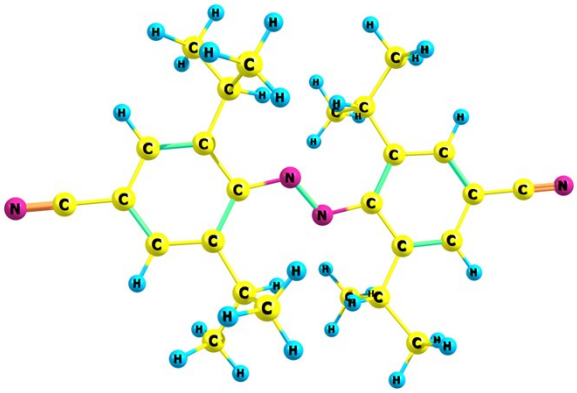

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| H | -1.216615000 | 3.864465000 | 1.684607000 |
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| H | -2.611165000 | -3.765700000 | -1.187987000 |
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| H | -0.458170000 | -1.697144000 | 1.944746000 |
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| C | 4.587681000 | 0.292034000 | 0.131478000 |
| H | 0.612647000 | 2.406946000 | 0.408910000 |
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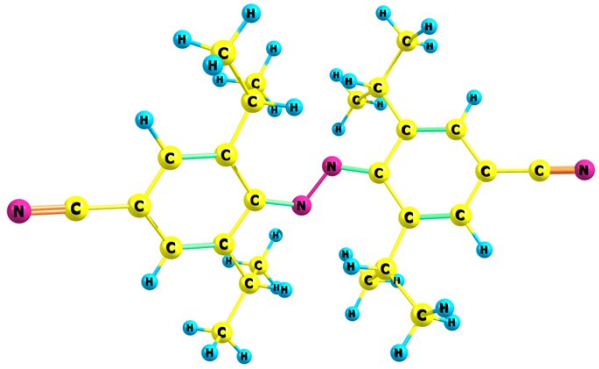
**$1^{2-}$**



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| C | 4.093528000 | -0.873960000 | -0.085124000 |
| H | 4.823418000 | -1.669684000 | 0.047252000 |
| C | 2.324076000 | -2.433852000 | 0.769903000 |
| H | 1.388012000 | -2.686677000 | 0.261714000 |
| C | 1.348912000 | 2.471269000 | -0.534927000 |
| H | 0.376166000 | 2.123102000 | -0.887325000 |
| C | 3.305810000 | -3.585034000 | 0.549653000 |
| H | 2.854050000 | -4.530328000 | 0.875966000 |
| H | 4.228337000 | -3.446836000 | 1.127768000 |
| H | 3.583776000 | -3.679444000 | -0.505774000 |
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| H | -1.063076000 | -4.300373000 | -1.655147000 |
| H | -2.100458000 | -3.116894000 | -2.483810000 |
| H | -2.732007000 | -4.070182000 | -1.129968000 |
| C | -1.135809000 | -3.093702000 | 0.850568000 |
| H | -0.694195000 | -2.351434000 | 1.520271000 |
| H | -0.465406000 | -3.964825000 | 0.807140000 |
| H | -2.100250000 | -3.420649000 | 1.262052000 |

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