# Electronic Supplementary Information

for

## A high-spin diradical dianion and its bridged chemically switchable single-molecule magnet

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# Content

## Experimental Section

**General considerations.** All experiments were carried out under an atmosphere of dry nitrogen by using modified Schlenk line or glovebox techniques. Toluene, THF and n-hexane were freshly distilled over Na/benzophenone and degassed three times before using. Elemental analyses were performed on an Elementar Vario EL III instrument at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences. EPR spectra were obtained on Bruker plus-6/1 X-band variable-temperature apparatus. Considering the $^{57}$Fe Mössbauer spectroscopic studied, the solid sample was the as-isolated complex, and it was placed into a Delrin Mössbauer sample cup for measurements and loaded under liquid nitrogen. The spectrum was recorded on a conventional spectrometer with alternating constant acceleration of the $\gamma$-source ($^{57}$Co/Rh, 1.8 GBq) at room temperature. Magnetic measurements were performed using a Quantum Design SQUID VMS magnetometer. For the single-crystal X-ray diffraction analyses, the data were collected on Bruker D8 CMOS detectors at 193 K. The structures were solved by direct methods and all refined on $F^2$ with the SHELX-2018/3 software package. The positions of the H atoms were calculated and considered isotropically according to a riding model. Commercially available reagents were purchased from Energy Chemical and Alfa-Assar, and used as received. 2,7-*t*Bu$_2$-PTO,[1] LMg-MgL[2] and LFe(Tol)[3] were synthesized according to the reported literatures.

**Synthesis of 1.** A mixture of 2,7-*t*Bu$_2$-PTO (136.4 mg, 0.36 mmol) and LMg-MgL (338.1 g, 0.38 mmol) in toluene (ca. 60 ml) was stirred at room temperature in an $N_2$-filled glovebox for 12 h to give a deep green solution. The solution was filtered, the filtrate was concentrated to ca. 10 mL and stored at –20 °C for 24 h to afford deep green crystals of **1** (185.2 mg, 40.4%). M.p. > 300 °C. Elemental analysis (%) Calcd for $C_{82}H_{104}Mg_2N_4O_4$•2($C_7H_8$): C, 79.93; H, 8.38; N, 3.88; Found: C, 79.94; H, 8.41; N, 3.49.

**Synthesis of 2.** A mixture of 2,7-*t*Bu$_2$-PTO (59.2 mg, 0.16 mmol) and LFe(Tol) (188.33 mg, 0.33 mmol) in toluene (ca. 30 ml) was stirred at room temperature in an $N_2$-filled glovebox for 12 h to give a brownish-red solution. The solution was filtered, the filtrate was concentrated to ca. 10 mL and stored at –20 °C for 24 h affording red crystals of **2** (90.1 mg, 43.1 %). Decomposed at 289 °C. Elemental analysis (%) Calcd for $C_{82}H_{104}Fe_2N_4O_4$•2($C_7H_8$): C, 76.58; H, 8.03; N, 3.72. Found: C, 76.61; H, 8.04; N, 3.48.

**Synthesis of 1K$_2$.** A mixture of **1** (90.5 mg, 0.07 mmol) and potassium (6.3 mg, 0.16 mmol) in THF (≈ 40 ml) was stirred at room temperature in an $N_2$-filled glovebox, whereupon the color of the solution was changed from deep green to light green. After stirring for 12 h, the solution was filtered, and the filtrate was concentrated to ca. 10 mL and stored at –20 °C for 24 h yielding light green crystals of **1K$_2$.** Removing all the volatiles in vacuo, the light green crystals soon became a light green powder (32 mg, 33.2 %). Decomposed at 170-173 °C. $^1$H NMR (400 MHz, $C_6D_6$): $\delta$ = 8.42 (s, 4H, Ar-*H*), 6.77 (d, *J* = 7.6 Hz, 8H, Ar-*H*), 6.57 (t, *J* = 7.6 Hz, 4H, Ar-*H*), 5.10 (s, 2H, $\gamma$-H), 3.72 (m, 8H, C*H*($CH_3$)$_2$), 3.56 (br, 16H, THF-OC*H*$_2$), 3.30 (m, 3H), 2.98 (m, 2H), 1.82 (s, 15H, C*H*$_3$), 1.80 (s, 10H, C*H*$_3$), 1.56 (m, 22H, C*H*$_3$), 1.40 (br, 16H, OCH$_2$C*H*$_2$), 1.22-1.15 (m, 38H, C*H*$_3$) ppm. $^{13}$C NMR (101 MHz, THF-$d_8$): $\delta$ = 167.72, 161.77, 147.16, 146.77, 144.37, 144.14, 142.91, 129.46, 125.85, 124.48, 123.69, 123.54, 110.97, 108.66, 94.32, 94.02,

68.02, 32.65, 28.87, 28.61, 26.19, 24.80, 24.56, 23.56, 23.27, 20.71 ppm. Elemental analysis (%) Calcd for $C_{82}H_{104}K_2Mg_2N_4O_4$•6($C_4H_8O$): C, 71.96; H, 8.66; N, 3.17; Found: C, 71.94; H, 8.01; N, 3.81.

**Synthesis of $2K_2$.** A mixture of **2** (120 mg, 0.09 mmol) and potassium (8.3 mg, 0.21 mmol) in THF (ca. 30 ml) was stirred at room temperature in an $N_2$-filled glovebox for 24 h, whereupon the color of the solution was changed from brownish red to brown. The solution was filtered, and the filtrate was concentrated to ca. 12 mL and stored at –20 °C for 24 h affording brown crystals of **$2K_2$.** Removing all the volatiles in vacuo, the crystals soon became a reddish brown powder (73 mg, 57.3 %). M.P. > 300 °C. Elemental analysis (%) Calcd for $C_{82}H_{104}Fe_2K_2N_4O_4$ •2($C_4H_8O$): C, 70.02; H, 7.83; N, 3.63. Found: C, 68.99; H, 7.70; N, 3.66.

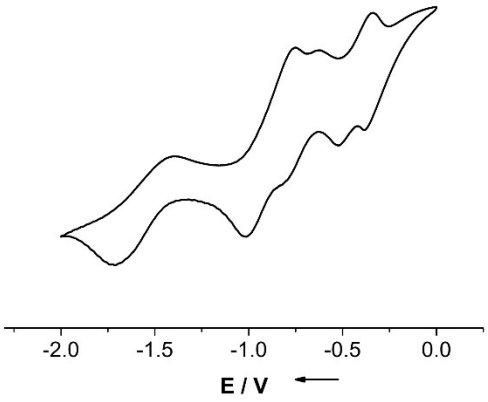


**Fig. S1** Cyclic voltammogram of 2,7-*t*$Bu_2$-PTO in THF ($1 \times 10^{-4}$ M, 0.1 M $^{n}Bu_4NPF_6$, Ag/Ag+ electrode, 298 K) was measured at 100 $mV \cdot s^{-1}$.

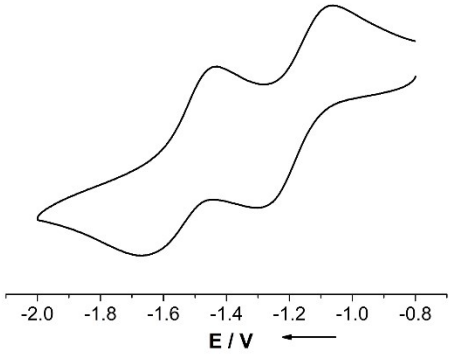


**Fig. S2** Cyclic voltammogram of **1** in THF ($1 \times 10^{-4}$ M, 0.1 M $^{n}Bu_4NPF_6$, Ag/Ag+ electrode, 298 K) was measured at 100 $mV \cdot s^{-1}$.

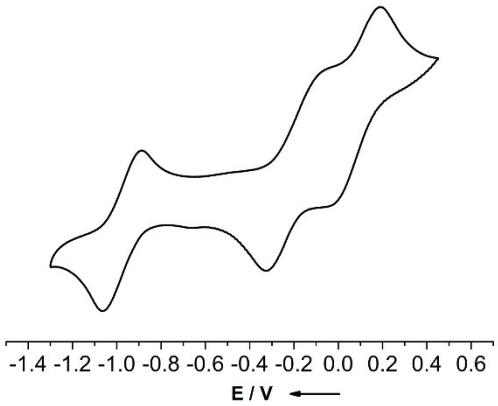


**Fig. S3** Cyclic voltammogram of **2** in THF ($1 \times 10^{-4}$ M, 0.1 M $^{n}Bu_4NPF_6$, $Ag/Ag^{+}$ electrode, 298 K) was measured at 100 $mV \cdot s^{-1}$.

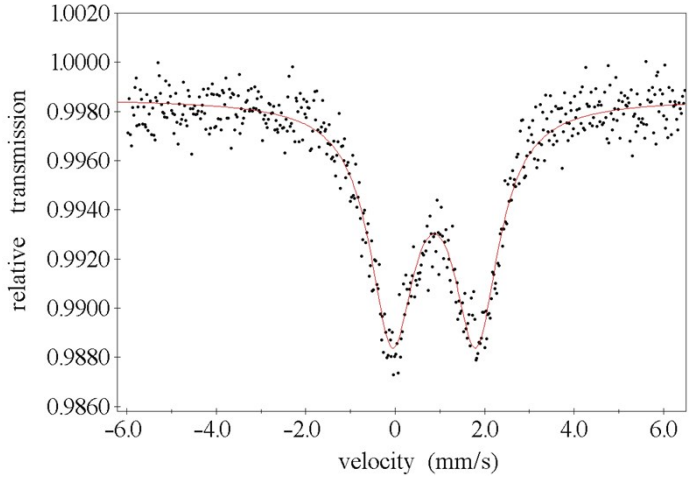


**Fig. S4** Zero-field $^{57}Fe$ Mössbauer spectrum of **2** recorded at 80K.

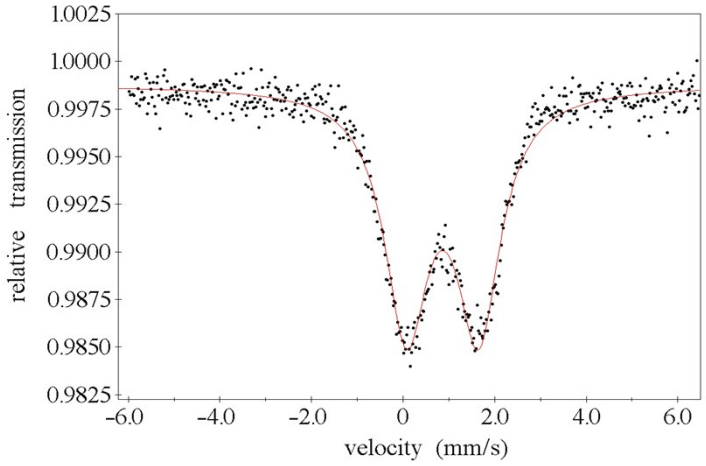


**Fig. S5** Zero-field $^{57}$Fe Mössbauer spectrum of **2K$_2$** recorded at 80K.

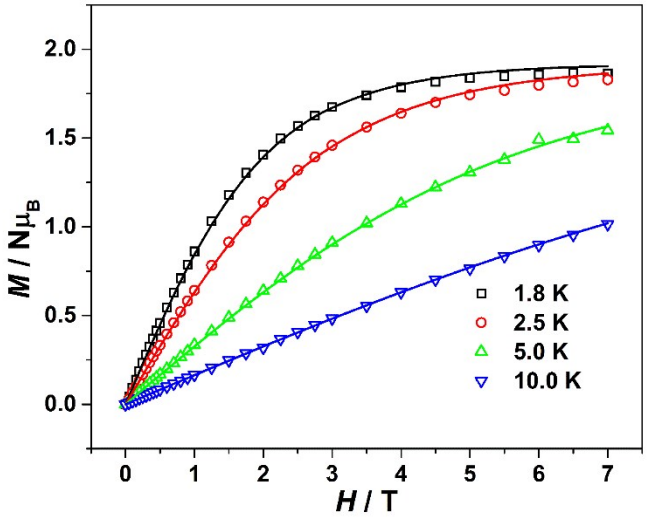


**Fig. S6** Isothermal magnetization at different temperatures for **1**. The solid lines are the best fitting results using PHI program.

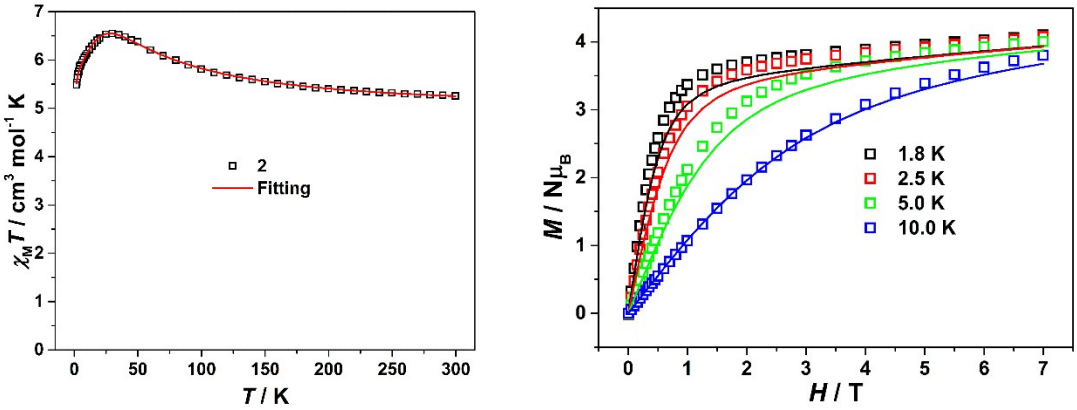


**Fig. S7** $\chi_M T$-$T$ (left) and $M$-$H$ (right) plots of **2** with the fitting result (solid line) using the PHI program, in which the constant $J$ between radicals is fixed at 165 cm$^{-1}$ same as that in compound **1** for comparison due to the very similar structure.

The temperature and field dependent magnetizations were fitted to quantify the anisotropy parameters based on equation 1 using the *PHI* program:

$$\hat{H} = -2J_1(\hat{S}_{Fe1}\hat{S}_{Rad1} + \hat{S}_{Rad2}\hat{S}_{Fe2}) - 2J\hat{S}_{Rad1}\hat{S}_{Rad2} - 2J_2(\hat{S}_{Fe1}\hat{S}_{Rad2} + \hat{S}_{Rad1}\hat{S}_{Fe2}) + D\left[\hat{S}_z^2 - \frac{S(S+1)}{3}\right] + g\mu_B\hat{S}H \quad (1)$$

where $J_1$ and $J_2$ are the magnetic coupling constants between the spins of radicals and Fe$^{II}$ ions (Fig. 7, inset). A reasonable fitting gives $D$ = –12.00(1) cm$^{-1}$, $g$ = 2.25(1), $J_1$ = –1092.5, $J$ = 165 (fixed), $J_2$ = –2.51(4) and $TIP$ = 5.93 × 10$^{-4}$ cm$^3$ mol$^{-1}$.

We can find that the fitting results for the $M$-$H$ curves show a large deviation with the experimental data. It can be ascribed to the electronic structure change from **1** to **2**. For example, the angle O1-Mg1-O2 is 83.87° in **1** but 80.97° in **2**. These reduced angle will lead to maximum electron cloud orientation shifts in radicals and the overlap decrease of the magnetic orbitals. Such that, the coupling between radicals may be weakened somewhat. So, the results in text are thought to be acceptable rather than here, although the fittings of $\chi_M T$-$T$ here are as beautiful as in the maintext.

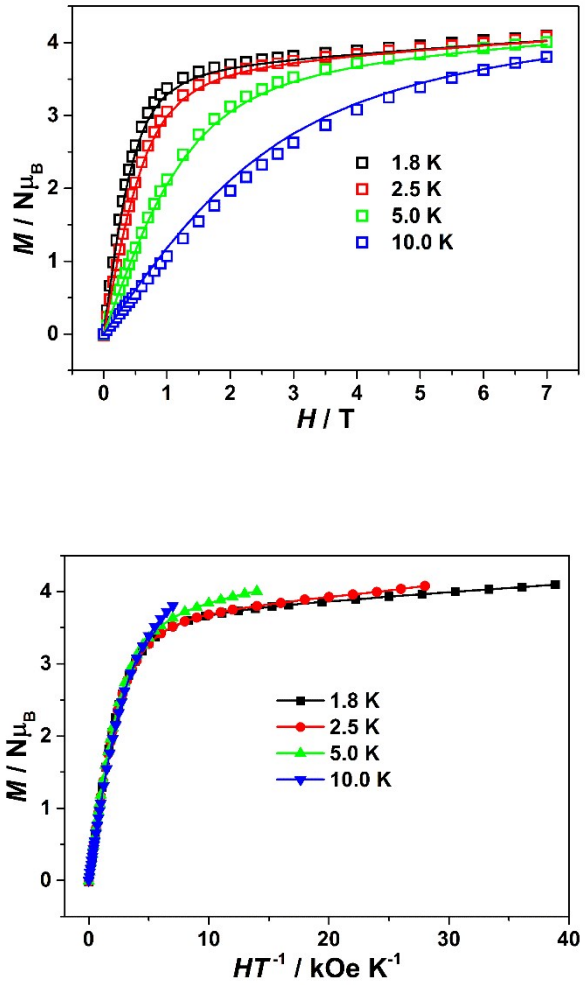


**Fig. S8** Top: Isothermal magnetization at different temperatures for **2**. The solid line is the fitting value; Down: Experimental *M vs H/T* plots at different temperatures for **2**.

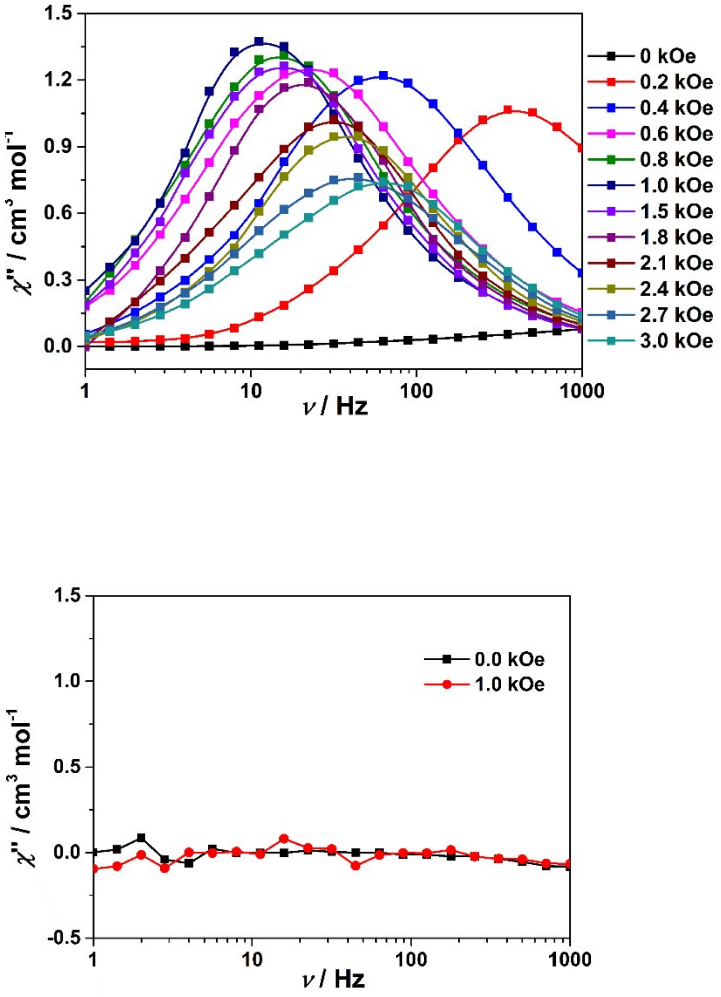


**Fig. S9** Isothermal field sweep measurement performed on polycrystalline sample of complex **2** (up) and **2K$_2$** (down).

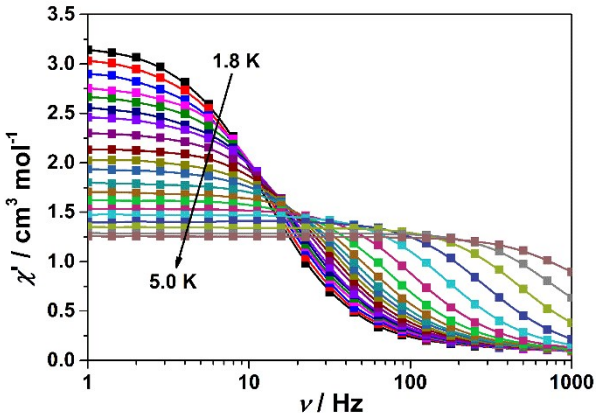


**Fig. S10** Frequency-dependence of the in-phase ($\chi_M'$) *ac*-susceptibilities for **2** at different temperatures (1.8 to 5.0 K).

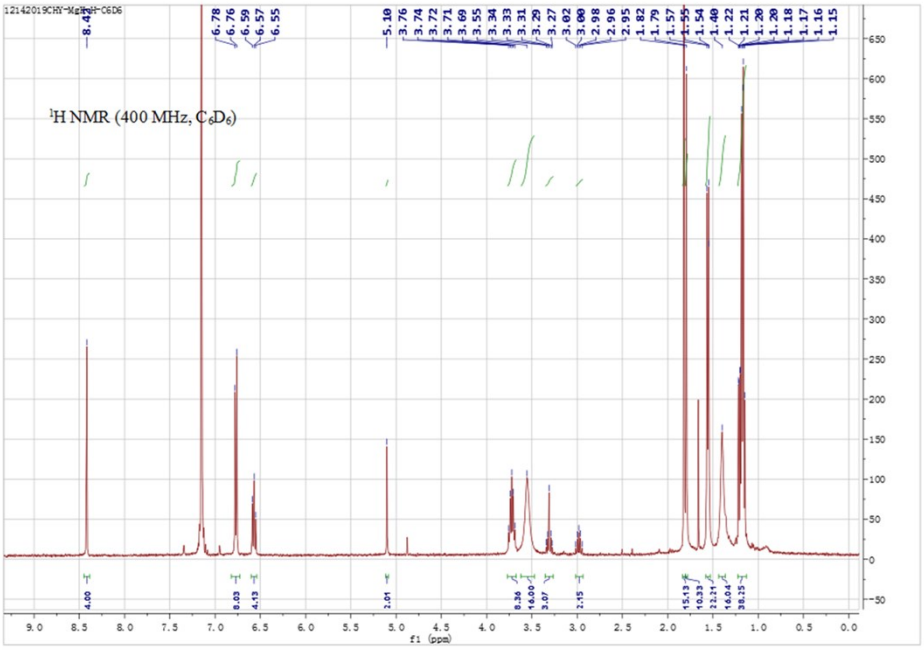


**Fig. S11** $^1$H NMR spectrum of **1K$_2$** in $C_6D_6$ at room temperature.

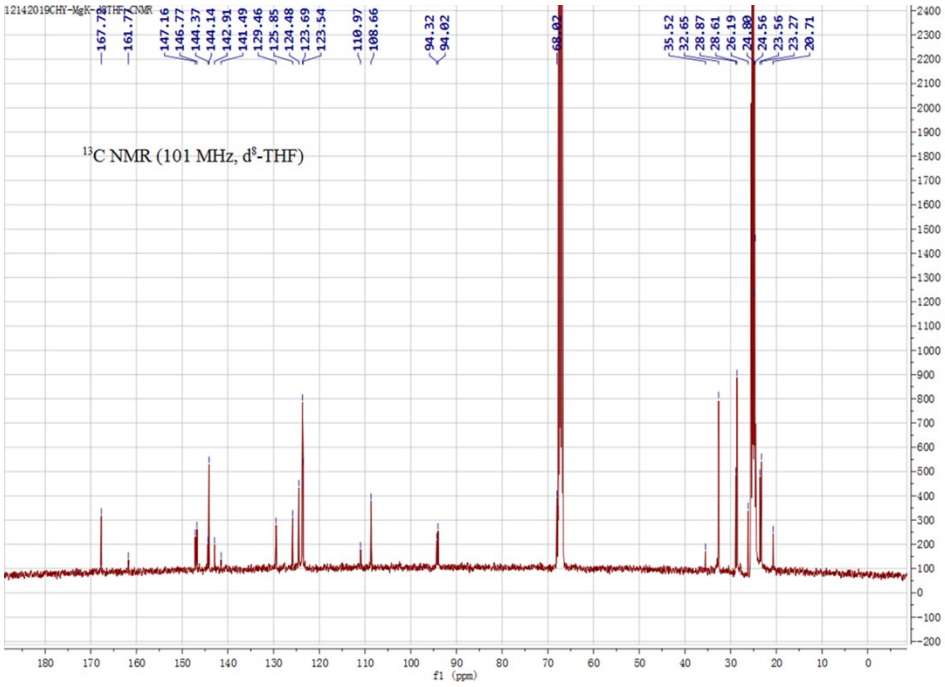


**Fig. S12** $^{13}$C NMR spectrum of **1K$_2$** in d$^8$-THF at room temperature.

**Table S1** Crystal data and structure refinements. Severely disordered solvent molecules in the four crystals were squeezed.

| | **1** | **1K$_2$** | **2** | **2K$_2$** |
|---|---|---|---|---|
| Formula | $C_{82}H_{104}Mg_2N_4O_4$ • $C_{14}H_{16}$ | $C_{82}H_{104}Mg_2K_2N_4O_4$ • 4($C_4H_8O$) | $C_{82}H_{104}Fe_2N_4O_4$ | $C_{82}H_{104}Fe_2K_2N_4O_4$ •4($C_4H_8O$) |
| Formula weight | 1442.57 | 1624.92 | 1321.39 | 1688.00 |
| Temp. (K) | 193(2) | 296(2) | 193(2) | 296(2) |
| Crystal system | Monoclinic | Triclinic | Monoclinic | Triclinic |
| Space group | *P* 21/*n* | *P*-1 | *P* 21/*n* | *P*-1 |
| *a* (Å) | 13.0089(3) | 12.3217(14) | 12.9263(5) | 13.1826(7) |
| *b* (Å) | 18.5762(4) | 14.4239(17) | 18.6784(6) | 13.9086(7) |
| *c* (Å) | 19.9212(5) | 15.785(2) | 19.8163(7) | 19.5230(11) |
| *α* (°) | 90 | 90.292(4) | 90 | 92.382(2) |
| *β* (°) | 101.5820(10) | 93.572(5) | 100.993(2) | 107.892(2) |
| γ (°) | 90 | 92.232(4) | 90 | 116.504(2) |
| *V* [Å$^3$] | 4716.05(19) | 2797.8(6) | 4696.7(3) | 2980.6(3) |
| *Z* | 2 | 1 | 2 | 1 |
| $\rho_{calcd}$ (g·cm$^{-3}$) | 1.016 | 0.964 | 0.934 | 0.940 |
| $\mu$ (mm$^{-1}$) | 0.376 | 0.142 | 1.910 | 0.357 |
| *F*(000) | 1560 | 878 | 1416 | 906 |
| Collected data | 33139 | 21163 | 33952 | 21664 |
| Unique data | 8282 [*R*(int)=0.0624] | 9776 [*R*(int) = 0.0540] | 8279 [*R*(int)= 0.0522] | 10360 [*R*(int)=0.0380] |
| GOF on $F^2$ | 1.097 | 1.019 | 1.049 | 1.054 |
| Final *R* indexes [I > 2σ(I)] | $R_1$ = 0.0673 $wR_2$ = 0.1251 | $R_1$ = 0.0603 $wR_2$ = 0.1586 | $R_1$ = 0.0488 $wR_2$ = 0.1544 | $R_1$ = 0.0520 $wR_2$ = 0.1532 |
| *R* indexes (all data) | $R_1$ = 0.1221 $wR_2$ = 0.1374 | $R_1$ = 0.0870 $wR_2$ = 0.1756 | $R_1$ = 0.0739 $wR_2$ = 0.1686 | $R_1$ = 0.0609 $wR_2$ = 0.1616 |
| Completeness | 0.994 | 0.990 | 0.997 | 0.985 |

**Table S2** The fit parameters obtained from analyses of the ac susceptibilities of **2** under 1.0 kOe dc field.

| *T* / *K* | $\chi_T$ / cm$^3$ mol$^{-1}$ | $\chi_S$ /cm$^3$ mol$^{-1}$ | ln($\tau$ / s) | *a* | $R^2$ |
|---|---|---|---|---|---|
| 1.8 | 3.21573 | 0.10315 | -4.3924 | 0.08205 | 0.01167 |
| 1.9 | 3.08632 | 0.10317 | -4.47789 | 0.08539 | 0.00733 |
| 2 | 2.94477 | 0.10424 | -4.57138 | 0.08637 | 0.00497 |
| 2.1 | 2.80046 | 0.10893 | -4.68429 | 0.07571 | 0.00896 |
| 2.2 | 2.697 | 0.10748 | -4.76074 | 0.08127 | 0.00679 |
| 2.3 | 2.58363 | 0.10592 | -4.84572 | 0.08285 | 0.00608 |
| 2.4 | 2.48313 | 0.10953 | -4.93303 | 0.07604 | 0.00749 |
| 2.6 | 2.32297 | 0.10759 | -5.08536 | 0.08163 | 0.00704 |
| 2.8 | 2.1637 | 0.10704 | -5.23846 | 0.07735 | 0.00693 |
| 3 | 2.03814 | 0.10611 | -5.39157 | 0.07952 | 0.00745 |
| 3.2 | 1.93825 | 0.10642 | -5.53091 | 0.0789 | 0.00724 |
| 3.4 | 1.81168 | 0.10625 | -5.70331 | 0.072 | 0.00471 |
| 3.6 | 1.71163 | 0.10616 | -5.91042 | 0.06361 | 0.00561 |
| 3.8 | 1.62372 | 0.10013 | -6.18304 | 0.06141 | 0.00319 |
| 4 | 1.53993 | 0.1047 | -6.55372 | 0.04069 | 0.00167 |
| 4.2 | 1.47738 | 0.09343 | -7.00998 | 0.03939 | 0.00178 |
| 4.4 | 1.40842 | 0.08986 | -7.52761 | 0.02738 | 0.0016 |
| 4.6 | 1.34757 | 0.09915 | -8.05962 | 0.01936 | 7.54E-04 |
| 4.8 | 1.28868 | 0.08134 | -8.62206 | 0.01705 | 1.06E-03 |
| 5 | 1.25309 | 1.60E-14 | -9.23172 | 0.03985 | 4.78E-04 |

## Computational details:

All the calculations were performed at Gaussian 09 program suite.[4,5] The ground-state structures of the studied compound **1** were optimized using density functional theory (DFT) at the (U)B3LYP/6-31G(d) level of approximation, and no imaginary frequency was found, which confirmed the local minimum of the optimized structures.

### Coordinates of complex 1

### Close-shell singlet state

| | | | |
|---|---|---|---|
| Mg | 0.3376 | 11.0548 | 11.0804 |
| N | 1.6182 | 10.5059 | 9.5145 |
| N | 1.6581 | 12.582 | 11.6408 |
| O | -0.448 | 11.0178 | 12.9651 |
| O | -0.5313 | 9.2036 | 11.0973 |
| C | -1.0128 | 9.9089 | 13.2541 |
| C | -1.0621 | 8.9082 | 12.2209 |
| C | -1.7078 | 7.6417 | 12.4765 |
| C | -1.7497 | 6.6428 | 11.4952 |
| H | -1.3218 | 6.798 | 10.6603 |
| C | -2.3984 | 5.4327 | 11.7064 |
| C | -3.0098 | 5.2252 | 12.9391 |
| H | -3.4702 | 4.4095 | 13.0973 |
| C | -2.9634 | 6.1895 | 13.9502 |
| C | -2.3162 | 7.414 | 13.737 |
| C | -2.4018 | 4.3715 | 10.5888 |
| C | -3.2417 | 3.182 | 10.9624 |
| H | -4.1739 | 3.4624 | 11.0736 |
| H | -2.9115 | 2.7987 | 11.8004 |
| H | -3.1881 | 2.5089 | 10.2527 |
| C | -2.912 | 4.9924 | 9.3007 |
| H | -2.947 | 4.3082 | 8.5995 |
| H | -2.3094 | 5.7131 | 9.0242 |
| H | -3.8108 | 5.3551 | 9.446 |
| C | -0.9655 | 3.9043 | 10.3525 |
| H | -0.5875 | 3.5716 | 11.1933 |
| H | -0.4269 | 4.655 | 10.0247 |
| H | -0.9614 | 3.1852 | 9.6855 |
| C | 2.5004 | 11.3738 | 8.992 |
| C | 2.8151 | 12.6188 | 9.5276 |
| C | 2.5173 | 13.1288 | 10.7886 |
| C | 1.5302 | 9.2245 | 8.9646 |
| C | 0.6949 | 8.9252 | 7.8413 |
| C | 0.6904 | 7.5266 | 7.4765 |
| H | 0.2004 | 7.2763 | 6.704 |
| C | 1.3109 | 6.5826 | 8.1292 |
| H | 1.1842 | 5.675 | 7.8784 |
| C | 2.1107 | 6.8867 | 9.1553 |
| H | 2.6208 | 6.2136 | 9.5886 |
| C | 2.184 | 8.2108 | 9.5715 |
| C | -0.1295 | 10.0561 | 7.2 |
| H | 0.169 | 10.9335 | 7.5762 |
| C | 0.0901 | 10.0624 | 5.6636 |
| H | 0.9201 | 9.5856 | 5.4499 |
| H | 0.152 | 10.9874 | 5.3473 |

| | | | |
|---|---|---|---|
| H | -0.6648 | 9.6157 | 5.2247 |
| C | -1.6195 | 9.8327 | 7.5563 |
| H | -2.1809 | 10.3887 | 6.9748 |
| H | -1.7722 | 10.0782 | 8.4912 |
| H | -1.8488 | 8.8887 | 7.4252 |
| C | 3.0427 | 8.4152 | 10.7971 |
| H | 2.6625 | 9.2182 | 11.2589 |
| C | 3.1039 | 7.3524 | 11.8432 |
| H | 2.2448 | 7.3064 | 12.3135 |
| H | 3.8152 | 7.563 | 12.4845 |
| H | 3.2912 | 6.4876 | 11.4213 |
| C | 4.49 | 8.7937 | 10.4465 |
| H | 5.0032 | 8.9267 | 11.2703 |
| H | 4.4934 | 9.6221 | 9.9221 |
| H | 4.8977 | 8.073 | 9.9221 |
| C | 1.658 | 13.0417 | 13.0118 |
| C | 0.7231 | 14.0221 | 13.3995 |
| C | 0.7434 | 14.3484 | 14.8104 |
| H | 0.1497 | 15.012 | 15.141 |
| C | 1.6069 | 13.7148 | 15.6883 |
| H | 1.5686 | 13.9207 | 16.6147 |
| C | 2.4786 | 12.831 | 15.2551 |
| H | 3.0883 | 12.443 | 15.8707 |
| C | 2.534 | 12.4414 | 13.8983 |
| C | -0.2271 | 14.6382 | 12.4959 |
| H | -0.0915 | 14.2549 | 11.581 |
| C | -1.6802 | 14.3404 | 12.9463 |
| H | -1.8745 | 14.8346 | 13.77 |
| H | -1.7814 | 13.379 | 13.1087 |
| H | -2.3036 | 14.6208 | 12.2422 |
| C | -0.052 | 16.1714 | 12.4161 |
| H | -0.8753 | 16.6101 | 12.7154 |
| H | 0.1397 | 16.4312 | 11.4926 |
| H | 0.6916 | 16.4454 | 12.9947 |
| C | 3.5349 | 11.4435 | 13.4804 |
| H | 3.3868 | 11.2408 | 12.513 |
| C | 3.4218 | 10.1463 | 14.2603 |
| H | 3.5389 | 10.3285 | 15.218 |
| H | 4.1143 | 9.5223 | 13.961 |
| H | 2.5377 | 9.7504 | 14.1121 |
| C | 4.9691 | 11.9821 | 13.6446 |
| H | 5.0658 | 12.8136 | 13.1344 |
| H | 5.6078 | 11.3184 | 13.3111 |
| H | 5.1465 | 12.1579 | 14.5909 |
| O | -4.1252 | 4.821 | 15.5384 |
| O | -4.0419 | 6.6352 | 17.4062 |
| C | -3.5604 | 5.9299 | 15.2494 |
| C | -3.511 | 6.9306 | 16.2826 |
| C | -2.8654 | 8.1971 | 16.0269 |
| C | -2.8234 | 9.196 | 17.0083 |
| H | -3.2514 | 9.0408 | 17.8432 |
| C | -2.1747 | 10.4061 | 16.7971 |
| C | -1.5633 | 10.6136 | 15.5643 |
| H | -1.103 | 11.4293 | 15.4061 |
| C | -1.6098 | 9.6493 | 14.5533 |
| C | -2.257 | 8.4248 | 14.7665 |

| | | | |
|---|---|---|---|
| C | -2.1713 | 11.4673 | 17.9147 |
| C | -1.3315 | 12.6568 | 17.541 |
| H | -0.3993 | 12.3764 | 17.4299 |
| H | -1.6616 | 13.0401 | 16.703 |
| H | -1.3851 | 13.3299 | 18.2508 |
| C | -1.6612 | 10.8464 | 19.2028 |
| H | -1.6262 | 11.5306 | 19.904 |
| H | -2.2638 | 10.1257 | 19.4793 |
| H | -0.7624 | 10.4837 | 19.0574 |
| C | -3.6077 | 11.9345 | 18.151 |
| H | -3.9856 | 12.2672 | 17.3102 |
| H | -4.1462 | 11.1838 | 18.4788 |
| H | -3.6118 | 12.6536 | 18.818 |
| Mg | -4.9108 | 4.784 | 17.423 |
| N | -6.1913 | 5.3329 | 18.989 |
| N | -6.2313 | 3.2568 | 16.8627 |
| C | -7.0736 | 4.465 | 19.5115 |
| C | -7.3883 | 3.22 | 18.9759 |
| C | -7.0905 | 2.71 | 17.7149 |
| C | -6.1033 | 6.6143 | 19.5388 |
| C | -5.2681 | 6.9136 | 20.6622 |
| C | -5.2636 | 8.3122 | 21.027 |
| H | -4.7736 | 8.5625 | 21.7995 |
| C | -5.8841 | 9.2562 | 20.3743 |
| H | -5.7574 | 10.1638 | 20.6251 |
| C | -6.6839 | 8.9521 | 19.3482 |
| H | -7.194 | 9.6252 | 18.9149 |
| C | -6.7571 | 7.628 | 18.932 |
| C | -4.4436 | 5.7827 | 21.3035 |
| H | -4.7422 | 4.9053 | 20.9272 |
| C | -4.6632 | 5.7764 | 22.8398 |
| H | -5.4932 | 6.2532 | 23.0536 |
| H | -4.7251 | 4.8514 | 23.1562 |
| H | -3.9083 | 6.2231 | 23.2788 |
| C | -2.9537 | 6.0061 | 20.9472 |
| H | -2.3923 | 5.4501 | 21.5287 |
| H | -2.8009 | 5.7606 | 20.0123 |
| H | -2.7244 | 6.9501 | 21.0783 |
| C | -7.6158 | 7.4236 | 17.7064 |
| H | -7.2357 | 6.6206 | 17.2446 |
| C | -7.6771 | 8.4864 | 16.6603 |
| H | -6.818 | 8.5324 | 16.19 |
| H | -8.3884 | 8.2758 | 16.0189 |
| H | -7.8644 | 9.3512 | 17.0821 |
| C | -9.0631 | 7.0451 | 18.0569 |
| H | -9.5764 | 6.9121 | 17.2332 |
| H | -9.0666 | 6.2167 | 18.5814 |
| H | -9.4709 | 7.7658 | 18.5814 |
| C | -6.2311 | 2.7971 | 15.4916 |
| C | -5.2963 | 1.8167 | 15.104 |
| C | -5.3166 | 1.4904 | 13.6931 |
| H | -4.7229 | 0.8268 | 13.3624 |
| C | -6.1801 | 2.124 | 12.8152 |
| H | -6.1418 | 1.9181 | 11.8888 |
| C | -7.0517 | 3.0078 | 13.2484 |
| H | -7.6615 | 3.3958 | 12.6327 |

| | | | |
|---|---|---|---|
| C | -7.1071 | 3.3974 | 14.6052 |
| C | -4.346 | 1.2006 | 16.0075 |
| H | -4.4817 | 1.5839 | 16.9225 |
| C | -2.8929 | 1.4984 | 15.5572 |
| H | -2.6986 | 1.0042 | 14.7334 |
| H | -2.7918 | 2.4598 | 15.3947 |
| H | -2.2696 | 1.218 | 16.2612 |
| C | -4.5211 | -0.3326 | 16.0874 |
| H | -3.6978 | -0.7713 | 15.7881 |
| H | -4.7129 | -0.5924 | 17.0109 |
| H | -5.2648 | -0.6066 | 15.5087 |
| C | -8.108 | 4.3953 | 15.023 |
| H | -7.96 | 4.598 | 15.9904 |
| C | -7.995 | 5.6925 | 14.2432 |
| H | -8.1121 | 5.5103 | 13.2855 |
| H | -8.6875 | 6.3165 | 14.5425 |
| H | -7.1109 | 6.0884 | 14.3914 |
| C | -9.5423 | 3.8567 | 14.8589 |
| H | -9.639 | 3.0252 | 15.3691 |
| H | -10.181 | 4.5204 | 15.1923 |
| H | -9.7197 | 3.6809 | 13.9125 |
| H | 3.361 | 13.2744 | 8.8818 |
| C | 3.2355 | 14.4189 | 11.2261 |
| H | 4.2054 | 14.4574 | 10.7758 |
| H | 2.6639 | 15.2683 | 10.9152 |
| H | 3.3363 | 14.4273 | 12.2913 |
| C | 3.2212 | 10.9574 | 7.6964 |
| H | 2.6536 | 11.2862 | 6.851 |
| H | 4.1929 | 11.4046 | 7.6693 |
| H | 3.3179 | 9.8922 | 7.6686 |
| H | -7.9342 | 2.5644 | 19.6217 |
| C | -7.7945 | 4.8814 | 20.8071 |
| H | -8.7616 | 4.4248 | 20.8397 |
| H | -7.221 | 4.5631 | 21.6525 |
| H | -7.9017 | 5.9458 | 20.8292 |
| C | -7.8087 | 1.4199 | 17.2774 |
| H | -7.2456 | 0.5703 | 17.6028 |
| H | -8.7849 | 1.3894 | 17.7144 |
| H | -7.8947 | 1.4037 | 16.211 |

**Open-shell singlet state**

| | | | |
|---|---|---|---|
| Mg | 5.13954 | 0.00003 | -0.0208 |
| N | 6.52559 | -1.51878 | -0.02706 |
| N | 6.52547 | 1.51896 | -0.02534 |
| O | 3.61488 | 0.00077 | -1.34093 |
| O | 3.62518 | -0.0008 | 1.31377 |
| C | 2.47432 | 0.00041 | -0.73573 |
| C | 2.48038 | -0.00045 | 0.71736 |
| C | 1.22434 | -0.00085 | 1.44236 |
| C | 1.20549 | -0.00164 | 2.84373 |
| H | 2.16436 | -0.00194 | 3.35076 |
| C | 0.00939 | -0.00201 | 3.57788 |
| C | -1.18839 | -0.0016 | 2.85596 |
| H | -2.14489 | -0.00185 | 3.36325 |
| C | -1.21333 | -0.00084 | 1.45002 |
| C | 0.00179 | -0.00044 | 0.71742 |

| | | | |
|---|---|---|---|
| C | 0.0564 | -0.00284 | 5.11651 |
| C | -1.35063 | -0.00317 | 5.74323 |
| H | -1.92602 | -0.89055 | 5.45604 |
| H | -1.926 | 0.88454 | 5.45699 |
| H | -1.26581 | -0.00375 | 6.8357 |
| C | 0.8049 | -1.26579 | 5.6055 |
| H | 0.8557 | -1.27609 | 6.70107 |
| H | 1.83051 | -1.30722 | 5.22408 |
| H | 0.28989 | -2.1771 | 5.28078 |
| C | 0.80491 | 1.25959 | 5.60685 |
| H | 0.28991 | 2.17124 | 5.2831 |
| H | 1.83052 | 1.30141 | 5.22547 |
| H | 0.85571 | 1.26873 | 6.70243 |
| C | 7.8415 | -1.28339 | -0.03968 |
| C | 8.42729 | 0.00018 | -0.04704 |
| C | 7.8414 | 1.28369 | -0.03839 |
| C | 6.03179 | -2.87072 | -0.01539 |
| C | 5.73242 | -3.52179 | -1.23927 |
| C | 5.15311 | -4.79593 | -1.19731 |
| H | 4.9167 | -5.30136 | -2.1302 |
| C | 4.87342 | -5.42756 | 0.00994 |
| H | 4.4206 | -6.41559 | 0.01977 |
| C | 5.18167 | -4.78512 | 1.2045 |
| H | 4.96726 | -5.28199 | 2.14725 |
| C | 5.76204 | -3.51094 | 1.2211 |
| C | 6.02484 | -2.88881 | -2.59946 |
| H | 6.50968 | -1.92379 | -2.42317 |
| C | 6.9963 | -3.7458 | -3.43626 |
| H | 7.93207 | -3.94252 | -2.90122 |
| H | 7.24498 | -3.23335 | -4.37334 |
| H | 6.55546 | -4.71524 | -3.69682 |
| C | 4.73155 | -2.61644 | -3.39311 |
| H | 4.96898 | -2.15043 | -4.3578 |
| H | 4.0671 | -1.94286 | -2.84418 |
| H | 4.18695 | -3.54605 | -3.59813 |
| C | 6.08636 | -2.86535 | 2.56807 |
| H | 6.57392 | -1.90565 | 2.37157 |
| C | 4.81087 | -2.57528 | 3.38414 |
| H | 4.14001 | -1.90343 | 2.8407 |
| H | 5.07062 | -2.10077 | 4.33892 |
| H | 4.26424 | -3.49888 | 3.60977 |
| C | 7.06872 | -3.71947 | 3.39492 |
| H | 7.34136 | -3.19713 | 4.31979 |
| H | 7.9912 | -3.93045 | 2.84249 |
| H | 6.62627 | -4.68195 | 3.67754 |
| C | 6.03156 | 2.87085 | -0.01229 |
| C | 5.73281 | 3.52349 | -1.23548 |
| C | 5.15333 | 4.7975 | -1.19218 |
| H | 4.91732 | 5.3041 | -2.12454 |
| C | 4.87295 | 5.42756 | 0.01573 |
| H | 4.42004 | 6.41553 | 0.02659 |
| C | 5.18063 | 4.78361 | 1.20963 |
| H | 4.96573 | 5.27926 | 2.1529 |
| C | 5.76107 | 3.50944 | 1.22489 |
| C | 6.02589 | 2.89223 | -2.59633 |
| H | 6.51169 | 1.9275 | -2.42104 |

| | | | |
|---|---|---|---|
| C | 4.73283 | 2.61936 | -3.39019 |
| H | 4.18727 | 3.54866 | -3.5941 |
| H | 4.0691 | 1.94451 | -2.84195 |
| H | 4.97066 | 2.15469 | -4.35541 |
| C | 6.99642 | 3.75104 | -3.43232 |
| H | 6.5544 | 4.72009 | -3.69232 |
| H | 7.24593 | 3.23956 | -4.3697 |
| H | 7.93182 | 3.94863 | -2.89695 |
| C | 6.08488 | 2.86222 | 2.5712 |
| H | 6.5717 | 1.90234 | 2.3737 |
| C | 4.80923 | 2.5723 | 3.38707 |
| H | 4.26335 | 3.49606 | 3.61381 |
| H | 5.06871 | 2.09652 | 4.34129 |
| H | 4.13781 | 1.90157 | 2.84296 |
| C | 7.06797 | 3.71475 | 3.39881 |
| H | 7.99078 | 3.92513 | 2.8467 |
| H | 7.33992 | 3.19151 | 4.32338 |
| H | 6.62644 | 4.6775 | 3.68198 |
| O | -3.61486 | -0.00075 | 1.34079 |
| O | -3.62516 | 0.00062 | -1.3139 |
| C | -2.47429 | -0.00044 | 0.7356 |
| C | -2.48036 | 0.00034 | -0.7175 |
| C | -1.22433 | 0.00076 | -1.4425 |
| C | -1.20547 | 0.00154 | -2.84388 |
| H | -2.16433 | 0.00181 | -3.35091 |
| C | -0.00936 | 0.00196 | -3.57802 |
| C | 1.18842 | 0.00159 | -2.8561 |
| H | 2.14492 | 0.00189 | -3.36338 |
| C | 1.21335 | 0.0008 | -1.45016 |
| C | -0.00177 | 0.00037 | -0.71756 |
| C | -0.05636 | 0.00279 | -5.11665 |
| C | 1.35067 | 0.00314 | -5.74336 |
| H | 1.92604 | 0.89054 | -5.45616 |
| H | 1.92606 | -0.88455 | -5.4571 |
| H | 1.26587 | 0.00371 | -6.83582 |
| C | -0.80487 | 1.26573 | -5.60564 |
| H | -0.85565 | 1.27604 | -6.70122 |
| H | -1.8305 | 1.30714 | -5.22425 |
| H | -0.28989 | 2.17704 | -5.28091 |
| C | -0.80484 | -1.25965 | -5.607 |
| H | -0.28982 | -2.1713 | -5.28326 |
| H | -1.83046 | -1.30151 | -5.22564 |
| H | -0.85564 | -1.26878 | -6.70258 |
| Mg | -5.13954 | 0.00003 | 0.02068 |
| N | -6.52558 | 1.51882 | 0.02702 |
| N | -6.52547 | -1.51892 | 0.02545 |
| C | -7.84149 | 1.28344 | 0.04013 |
| C | -8.42728 | -0.00012 | 0.04749 |
| C | -7.84139 | -1.28364 | 0.0389 |
| C | -6.03177 | 2.87075 | 0.0152 |
| C | -5.73308 | 3.52238 | 1.23895 |
| C | -5.15365 | 4.79645 | 1.19672 |
| H | -4.91766 | 5.30227 | 2.12951 |
| C | -4.87333 | 5.42757 | -0.01065 |
| H | -4.42048 | 6.41557 | -0.02067 |
| C | -5.18099 | 4.78463 | -1.20509 |

| | | | |
|---|---|---|---|
| H | -4.96615 | 5.2811 | -2.14795 |
| C | -5.76132 | 3.51042 | -1.22144 |
| C | -6.02609 | 2.88995 | 2.59927 |
| H | -6.51217 | 1.92551 | 2.42319 |
| C | -6.99623 | 3.74825 | 3.43624 |
| H | -7.93161 | 3.94674 | 2.90116 |
| H | -7.24583 | 3.2359 | 4.37312 |
| H | -6.55384 | 4.71687 | 3.69721 |
| C | -4.73295 | 2.61603 | 3.39265 |
| H | -4.97072 | 2.15063 | 4.35754 |
| H | -4.06951 | 1.94145 | 2.84373 |
| H | -4.18709 | 3.54502 | 3.59721 |
| C | -6.08512 | 2.86432 | -2.56828 |
| H | -6.57157 | 1.90409 | -2.37159 |
| C | -4.80951 | 2.57561 | -3.38463 |
| H | -4.13779 | 1.90459 | -2.84124 |
| H | -5.06898 | 2.10063 | -4.33925 |
| H | -4.26396 | 3.49976 | -3.6106 |
| C | -7.06867 | 3.71727 | -3.39492 |
| H | -7.34048 | 3.19487 | -4.32 |
| H | -7.99152 | 3.92664 | -2.84251 |
| H | -6.6276 | 4.68052 | -3.67712 |
| C | -6.03157 | -2.87081 | 0.01237 |
| C | -5.73333 | -3.52379 | 1.2355 |
| C | -5.15382 | -4.79779 | 1.19207 |
| H | -4.91813 | -5.30462 | 2.12438 |
| C | -4.87304 | -5.42756 | -0.0159 |
| H | -4.42016 | -6.41554 | -0.02685 |
| C | -5.1803 | -4.78331 | -1.20974 |
| H | -4.96514 | -5.27875 | -2.15307 |
| C | -5.76063 | -3.50909 | -1.22489 |
| C | -6.0268 | -2.89286 | 2.5964 |
| H | -6.51347 | -1.92855 | 2.42123 |
| C | -4.73384 | -2.61891 | 3.39006 |
| H | -4.18742 | -3.54777 | 3.59368 |
| H | -4.07081 | -1.94337 | 2.84181 |
| H | -4.9719 | -2.15461 | 4.35542 |
| C | -6.99641 | -3.75256 | 3.43256 |
| H | -6.5533 | -4.72101 | 3.69293 |
| H | -7.2466 | -3.24108 | 4.36977 |
| H | -7.93152 | -3.95144 | 2.89716 |
| C | -6.08408 | -2.86158 | -2.57114 |
| H | -6.56998 | -1.90125 | -2.37356 |
| C | -4.80835 | -2.57288 | -3.38731 |
| H | -4.26341 | -3.49713 | -3.6143 |
| H | -5.06762 | -2.09676 | -4.34142 |
| H | -4.13616 | -1.90283 | -2.84331 |
| C | -7.06817 | -3.71324 | -3.39848 |
| H | -7.99125 | -3.92226 | -2.84632 |
| H | -7.33948 | -3.19001 | -4.32324 |
| H | -6.62777 | -4.67662 | -3.68125 |
| H | 9.51014 | 0.00023 | -0.05839 |
| C | 8.80879 | 2.45475 | -0.04338 |
| H | 9.84538 | 2.11256 | -0.05886 |
| H | 8.64186 | 3.09696 | -0.91408 |
| H | 8.66456 | 3.08512 | 0.84004 |

| | | | |
|---|---|---|---|
| C | 8.809 | -2.45436 | -0.04506 |
| H | 8.63945 | -3.09878 | -0.91357 |
| H | 9.8455 | -2.1121 | -0.06444 |
| H | 8.66758 | -3.0825 | 0.84043 |
| H | -9.51013 | -0.00017 | 0.05916 |
| C | -8.80896 | 2.45443 | 0.04685 |
| H | -9.84555 | 2.11214 | 0.06015 |
| H | -8.64321 | 3.09427 | 0.91954 |
| H | -8.66361 | 3.08721 | -0.83462 |
| C | -8.80878 | -2.4547 | 0.04503 |
| H | -8.64491 | -3.0932 | 0.91908 |
| H | -9.84542 | -2.11247 | 0.05567 |
| H | -8.66145 | -3.08881 | -0.83514 |

## Triplet state

| | | | |
|---|---|---|---|
| Mg | 0.3376 | 11.0548 | 11.0804 |
| N | 1.6182 | 10.5059 | 9.5145 |
| N | 1.6581 | 12.582 | 11.6408 |
| O | -0.448 | 11.0178 | 12.9651 |
| O | -0.5313 | 9.2036 | 11.0973 |
| C | -1.0128 | 9.9089 | 13.2541 |
| C | -1.0621 | 8.9082 | 12.2209 |
| C | -1.7078 | 7.6417 | 12.4765 |
| C | -1.7497 | 6.6428 | 11.4952 |
| H | -1.3218 | 6.798 | 10.6603 |
| C | -2.3984 | 5.4327 | 11.7064 |
| C | -3.0098 | 5.2252 | 12.9391 |
| H | -3.4702 | 4.4095 | 13.0973 |
| C | -2.9634 | 6.1895 | 13.9502 |
| C | -2.3162 | 7.414 | 13.737 |
| C | -2.4018 | 4.3715 | 10.5888 |
| C | -3.2417 | 3.182 | 10.9624 |
| H | -4.1739 | 3.4624 | 11.0736 |
| H | -2.9115 | 2.7987 | 11.8004 |
| H | -3.1881 | 2.5089 | 10.2527 |
| C | -2.912 | 4.9924 | 9.3007 |
| H | -2.947 | 4.3082 | 8.5995 |
| H | -2.3094 | 5.7131 | 9.0242 |
| H | -3.8108 | 5.3551 | 9.446 |
| C | -0.9655 | 3.9043 | 10.3525 |
| H | -0.5875 | 3.5716 | 11.1933 |
| H | -0.4269 | 4.655 | 10.0247 |
| H | -0.9614 | 3.1852 | 9.6855 |
| C | 2.5004 | 11.3738 | 8.992 |
| C | 2.8151 | 12.6188 | 9.5276 |
| C | 2.5173 | 13.1288 | 10.7886 |
| C | 1.5302 | 9.2245 | 8.9646 |
| C | 0.6949 | 8.9252 | 7.8413 |
| C | 0.6904 | 7.5266 | 7.4765 |
| H | 0.2004 | 7.2763 | 6.704 |
| C | 1.3109 | 6.5826 | 8.1292 |
| H | 1.1842 | 5.675 | 7.8784 |
| C | 2.1107 | 6.8867 | 9.1553 |
| H | 2.6208 | 6.2136 | 9.5886 |
| C | 2.184 | 8.2108 | 9.5715 |
| C | -0.1295 | 10.0561 | 7.2 |

| | | | |
|---|---|---|---|
| H | 0.169 | 10.9335 | 7.5762 |
| C | 0.0901 | 10.0624 | 5.6636 |
| H | 0.9201 | 9.5856 | 5.4499 |
| H | 0.152 | 10.9874 | 5.3473 |
| H | -0.6648 | 9.6157 | 5.2247 |
| C | -1.6195 | 9.8327 | 7.5563 |
| H | -2.1809 | 10.3887 | 6.9748 |
| H | -1.7722 | 10.0782 | 8.4912 |
| H | -1.8488 | 8.8887 | 7.4252 |
| C | 3.0427 | 8.4152 | 10.7971 |
| H | 2.6625 | 9.2182 | 11.2589 |
| C | 3.1039 | 7.3524 | 11.8432 |
| H | 2.2448 | 7.3064 | 12.3135 |
| H | 3.8152 | 7.563 | 12.4845 |
| H | 3.2912 | 6.4876 | 11.4213 |
| C | 4.49 | 8.7937 | 10.4465 |
| H | 5.0032 | 8.9267 | 11.2703 |
| H | 4.4934 | 9.6221 | 9.9221 |
| H | 4.8977 | 8.073 | 9.9221 |
| C | 1.658 | 13.0417 | 13.0118 |
| C | 0.7231 | 14.0221 | 13.3995 |
| C | 0.7434 | 14.3484 | 14.8104 |
| H | 0.1497 | 15.012 | 15.141 |
| C | 1.6069 | 13.7148 | 15.6883 |
| H | 1.5686 | 13.9207 | 16.6147 |
| C | 2.4786 | 12.831 | 15.2551 |
| H | 3.0883 | 12.443 | 15.8707 |
| C | 2.534 | 12.4414 | 13.8983 |
| C | -0.2271 | 14.6382 | 12.4959 |
| H | -0.0915 | 14.2549 | 11.581 |
| C | -1.6802 | 14.3404 | 12.9463 |
| H | -1.8745 | 14.8346 | 13.77 |
| H | -1.7814 | 13.379 | 13.1087 |
| H | -2.3036 | 14.6208 | 12.2422 |
| C | -0.052 | 16.1714 | 12.4161 |
| H | -0.8753 | 16.6101 | 12.7154 |
| H | 0.1397 | 16.4312 | 11.4926 |
| H | 0.6916 | 16.4454 | 12.9947 |
| C | 3.5349 | 11.4435 | 13.4804 |
| H | 3.3868 | 11.2408 | 12.513 |
| C | 3.4218 | 10.1463 | 14.2603 |
| H | 3.5389 | 10.3285 | 15.218 |
| H | 4.1143 | 9.5223 | 13.961 |
| H | 2.5377 | 9.7504 | 14.1121 |
| C | 4.9691 | 11.9821 | 13.6446 |
| H | 5.0658 | 12.8136 | 13.1344 |
| H | 5.6078 | 11.3184 | 13.3111 |
| H | 5.1465 | 12.1579 | 14.5909 |
| O | -4.1252 | 4.821 | 15.5384 |
| O | -4.0419 | 6.6352 | 17.4062 |
| C | -3.5604 | 5.9299 | 15.2494 |
| C | -3.511 | 6.9306 | 16.2826 |
| C | -2.8654 | 8.1971 | 16.0269 |
| C | -2.8234 | 9.196 | 17.0083 |
| H | -3.2514 | 9.0408 | 17.8432 |
| C | -2.1747 | 10.4061 | 16.7971 |

| | | | |
|---|---|---|---|
| C | -1.5633 | 10.6136 | 15.5643 |
| H | -1.103 | 11.4293 | 15.4061 |
| C | -1.6098 | 9.6493 | 14.5533 |
| C | -2.257 | 8.4248 | 14.7665 |
| C | -2.1713 | 11.4673 | 17.9147 |
| C | -1.3315 | 12.6568 | 17.541 |
| H | -0.3993 | 12.3764 | 17.4299 |
| H | -1.6616 | 13.0401 | 16.703 |
| H | -1.3851 | 13.3299 | 18.2508 |
| C | -1.6612 | 10.8464 | 19.2028 |
| H | -1.6262 | 11.5306 | 19.904 |
| H | -2.2638 | 10.1257 | 19.4793 |
| H | -0.7624 | 10.4837 | 19.0574 |
| C | -3.6077 | 11.9345 | 18.151 |
| H | -3.9856 | 12.2672 | 17.3102 |
| H | -4.1462 | 11.1838 | 18.4788 |
| H | -3.6118 | 12.6536 | 18.818 |
| Mg | -4.9108 | 4.784 | 17.423 |
| N | -6.1913 | 5.3329 | 18.989 |
| N | -6.2313 | 3.2568 | 16.8627 |
| C | -7.0736 | 4.465 | 19.5115 |
| C | -7.3883 | 3.22 | 18.9759 |
| C | -7.0905 | 2.71 | 17.7149 |
| C | -6.1033 | 6.6143 | 19.5388 |
| C | -5.2681 | 6.9136 | 20.6622 |
| C | -5.2636 | 8.3122 | 21.027 |
| H | -4.7736 | 8.5625 | 21.7995 |
| C | -5.8841 | 9.2562 | 20.3743 |
| H | -5.7574 | 10.1638 | 20.6251 |
| C | -6.6839 | 8.9521 | 19.3482 |
| H | -7.194 | 9.6252 | 18.9149 |
| C | -6.7571 | 7.628 | 18.932 |
| C | -4.4436 | 5.7827 | 21.3035 |
| H | -4.7422 | 4.9053 | 20.9272 |
| C | -4.6632 | 5.7764 | 22.8398 |
| H | -5.4932 | 6.2532 | 23.0536 |
| H | -4.7251 | 4.8514 | 23.1562 |
| H | -3.9083 | 6.2231 | 23.2788 |
| C | -2.9537 | 6.0061 | 20.9472 |
| H | -2.3923 | 5.4501 | 21.5287 |
| H | -2.8009 | 5.7606 | 20.0123 |
| H | -2.7244 | 6.9501 | 21.0783 |
| C | -7.6158 | 7.4236 | 17.7064 |
| H | -7.2357 | 6.6206 | 17.2446 |
| C | -7.6771 | 8.4864 | 16.6603 |
| H | -6.818 | 8.5324 | 16.19 |
| H | -8.3884 | 8.2758 | 16.0189 |
| H | -7.8644 | 9.3512 | 17.0821 |
| C | -9.0631 | 7.0451 | 18.0569 |
| H | -9.5764 | 6.9121 | 17.2332 |
| H | -9.0666 | 6.2167 | 18.5814 |
| H | -9.4709 | 7.7658 | 18.5814 |
| C | -6.2311 | 2.7971 | 15.4916 |
| C | -5.2963 | 1.8167 | 15.104 |
| C | -5.3166 | 1.4904 | 13.6931 |
| H | -4.7229 | 0.8268 | 13.3624 |

| | | | |
|---|---|---|---|
| C | -6.1801 | 2.124 | 12.8152 |
| H | -6.1418 | 1.9181 | 11.8888 |
| C | -7.0517 | 3.0078 | 13.2484 |
| H | -7.6615 | 3.3958 | 12.6327 |
| C | -7.1071 | 3.3974 | 14.6052 |
| C | -4.346 | 1.2006 | 16.0075 |
| H | -4.4817 | 1.5839 | 16.9225 |
| C | -2.8929 | 1.4984 | 15.5572 |
| H | -2.6986 | 1.0042 | 14.7334 |
| H | -2.7918 | 2.4598 | 15.3947 |
| H | -2.2696 | 1.218 | 16.2612 |
| C | -4.5211 | -0.3326 | 16.0874 |
| H | -3.6978 | -0.7713 | 15.7881 |
| H | -4.7129 | -0.5924 | 17.0109 |
| H | -5.2648 | -0.6066 | 15.5087 |
| C | -8.108 | 4.3953 | 15.023 |
| H | -7.96 | 4.598 | 15.9904 |
| C | -7.995 | 5.6925 | 14.2432 |
| H | -8.1121 | 5.5103 | 13.2855 |
| H | -8.6875 | 6.3165 | 14.5425 |
| H | -7.1109 | 6.0884 | 14.3914 |
| C | -9.5423 | 3.8567 | 14.8589 |
| H | -9.639 | 3.0252 | 15.3691 |
| H | -10.181 | 4.5204 | 15.1923 |
| H | -9.7197 | 3.6809 | 13.9125 |
| H | 3.361 | 13.2744 | 8.8818 |
| C | 3.2355 | 14.4189 | 11.2261 |
| H | 4.2054 | 14.4574 | 10.7758 |
| H | 2.6639 | 15.2683 | 10.9152 |
| H | 3.3363 | 14.4273 | 12.2913 |
| C | 3.2212 | 10.9574 | 7.6964 |
| H | 2.6536 | 11.2862 | 6.851 |
| H | 4.1929 | 11.4046 | 7.6693 |
| H | 3.3179 | 9.8922 | 7.6686 |
| H | -7.9342 | 2.5644 | 19.6217 |
| C | -7.7945 | 4.8814 | 20.8071 |
| H | -8.7616 | 4.4248 | 20.8397 |
| H | -7.221 | 4.5631 | 21.6525 |
| H | -7.9017 | 5.9458 | 20.8292 |
| C | -7.8087 | 1.4199 | 17.2774 |
| H | -7.2456 | 0.5703 | 17.6028 |
| H | -8.7849 | 1.3894 | 17.7144 |
| H | -7.8947 | 1.4037 | 16.211 |

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