Electronic Supplementary Information for

Temperature induced single-crystal to single-crystal transformation of uranium azide complexes

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1. Experimental Procedures

General information: All manipulations were performed under an N_2 atmosphere using standard Schlenk techniques or in an N_2 glovebox (<1 ppm O_2/H_2O). Solvents were dried and deoxygenated by distillation under nitrogen and further dried over 4 Å molecular sieves before use. THF-d_8 was dried over Na/K and stored under an N_2 atmosphere prior to use. Complex **1** was synthesized by reported procedure.[1] Other reagents were purchased and used without further purification. Nuclear magnetic resonance (NMR) spectroscopy was performed using a Bruker AVIII-400 (^{1}H 400 MHz; ^{31}P{^{1}H} 162 MHz) spectrometer. Absolute values of the coupling constants (δ) are provided in Hertz (Hz). Multiplicities of peaks are abbreviated as single (s), double (d), triplet (t), multiplet (m) or broad (br). Magnetic measurements on crystalline samples were performed using a Quantum Design SQUID VSM magnetometer from 370.0 to 1.8 K under an external magnetic field of 1000 Oe. Fourier transform infrared spectra (FT-IR) were measured on a Nicolet FTIR 170X spectrophotometer in the range of 2200-200 cm^{-1} at 25 °C using KBr plates. UV-vis-NIR absorption spectra were recorded on a Lambda 750 spectrometer at RT in THF. Elemental analyses (C, H, N) were performed on a Vario MICRO elemental analyser at the Center of Modern Analysis of Nanjing University.

Synthesis of complex 2

Complex **1** (71.5 mg, 0.1 mmol) and NaN_3 (13.0 mg, 0.2 mmol) were added to a 5 mL flask and dissolved in THF (2 mL). The mixture was stirred at RT for 10 h and then the solvent was removed and the residue was extracted with ether (3 mL). The filtrate was dried at 60 ℃ to afford complex **2** as a pure yellow solid (56.8 mg, 78%). Crystal of **2** compatible for X-ray diffraction were grown from a saturated solution in ether (2 mL) stored at 60 ℃. ^{1}H NMR (d_8-THF, 400 MHz, ppm, 60 ℃): 44.1 (s, 2H, CH_2), 30.8 (s, 2H, CH_2), 17.9 (s, 7H, CH(CH_3)$_2$), 5.1 (s, 6H, N(CH_3)$_2$), -58.8 (s, 7H, CH(CH_3)$_2$). ^{31}P{^{1}H} NMR (d_8-THF, 162 MHz, ppm): no signal was not observed in the range of +1000 ~ -1000 ppm. Anal. Calcd (%) for $C_{20}H_{48}N_{10}P_2U$: C, 32.97; H, 6.64; N, 19.22. Found: C, 32.71; H, 6.22; N, 18.69. FT-IR ν/cm^{-1} (KBr): 2953 (w), 2863 (w), 2777 (w), 2075 (s, terminal N_3^-), 1464 (w), 1351 (w), 1279 (w), 1235 (w), 1134 (w), 1017 (w), 939 (w), 877 (w), 777 (w), 646 (w), 604 (w), 528 (w).

Synthesis of complex 3

Complex **1** (71.5 mg, 0.1 mmol) and NaN_3 (13.0 mg, 0.2 mmol) were added to a 5 mL flask and dissolved in THF (2 mL). The mixture was stirred at RT for 10 h and then the solvent was removed under reduced pressure and the residue was extracted with ether (3 mL). The filtrate was stored at -20 ℃ to afford complex **2** as a green crystalloid (55.4 mg, 76%). ^{1}H NMR (d_8-THF, 400 MHz, ppm, -60 ℃): 82.1 (s, 2H, C*H*$_2$), 62.1 (s, 2H, C*H*$_2$), 40.8 (s, 2H, C*H*$_2$), 19.2 (s, 6H, CH(C*H*$_3$)$_2$), 18.6 (s, 2H, C*H*$_2$), 8.5 (s, 6H, CH(C*H*$_3$)$_2$), 5.5 (s, 6H, CH(C*H*$_3$)$_2$). 5.2 (s, 6H, CH(C*H*$_3$)$_2$). -2.9 (s, 6H, N(C*H*$_3$)$_2$). -19.7 (s, 2H, C*H*(CH$_3$)$_2$). -62.1 (s, 2H, C*H*(CH$_3$)$_2$). -76.3 (s, 6H, N(C*H*$_3$)$_2$). ^{31}P{^{1}H} NMR (d_8-THF, 162 MHz, ppm): no signal was not observed in the range of +1000 ~ -1000 ppm. Anal. Calcd (%) for $C_{40}H_{96}N_{20}P_4U_2$: C, 32.97; H, 6.64; N, 19.22. Found: C, 32.80; H, 6.56; N, 19.08. FT-IR ν/cm^{-1} (KBr): 2964 (w), 2869 (w), 2824 (w), 2770 (w), 2134 (w, bridged N_3^-), 2079 (s, terminal N_3^-), 1466 (w), 1362 (w), 1280 (w), 1236 (w), 1128 (w), 1024 (w), 933 (w), 875 (w), 770 (w), 699 (w), 645 (w), 600 (w), 523 (w).

Synthesis of complex 4

Method A: Complex **2** (72.9 mg, 0.1 mmol) and KC_8 (27.2 mg, 0.2 mmol) were added to a 5 mL flask and dissolved in THF (2 mL). The mixture was stirred at RT for 6 h and then the solvent was removed under reduced pressure and the residue was extracted with ether (3 mL). The filtrate was dried to afford complex **4** as a pure brownish solid (44.2 mg, 67%). *Method B*: Complex **3** (145.7 mg, 0.1 mmol) and KC_8 (54.4 mg, 0.4 mmol) were added to a 5 mL flask and dissolved in THF (3 mL). The mixture was stirred at RT for 6 h and then the solvent was removed under reduced pressure and the residue was extracted with ether (3 mL). The filtrate was dried to afford complex **6** as a pure brownish solid (85.8 mg, 65%). Crystal of **4** compatible for X-ray diffraction were grown from a saturated solution in ether (2 mL) stored at RT for one day. ^{1}H NMR (d_8-THF, 400 MHz, ppm, RT): 7.6 (s, 12H, CH(C*H*$_3$)$_2$), -10.2 (s, 8H, C*H*$_2$), -16.6 (s, 12H, CH(C*H*$_3$)$_2$), -26.5 (s, 4H, C*H*(CH$_3$)$_2$), -30.1 (s, 12H, N(C*H*$_3$)$_2$). ^{31}P{^{1}H} NMR (d_8-THF, 162 MHz, ppm): no signal was not observed in the range of +1000 ~ -1000 ppm. Anal. Calcd (%) for $C_{40}H_{96}N_{10}P_4U_2$: C, 36.47; H, 7.35; N, 10.63. Found: C, 36.67; H, 7.13; N, 10.54.

2. Supporting Figures

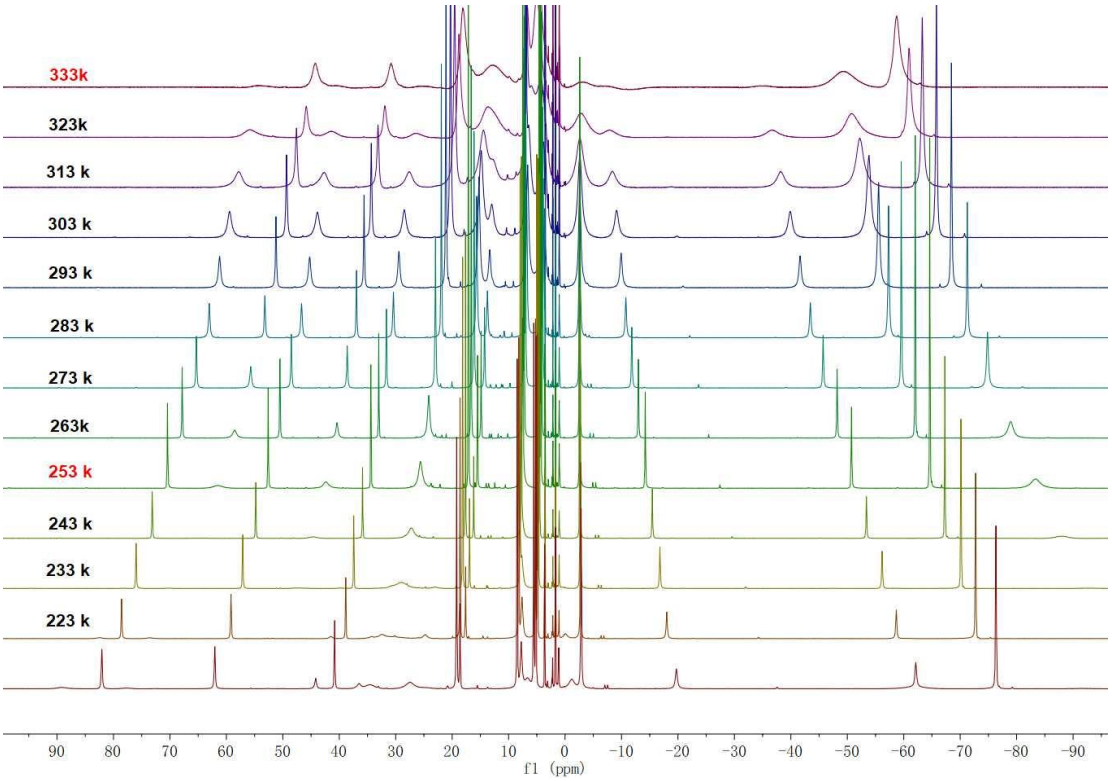


Figure S1. Variable-temperature ^{1}H NMR spectrum (from 333 K to 213 K) of complex **2** in d_8-THF.

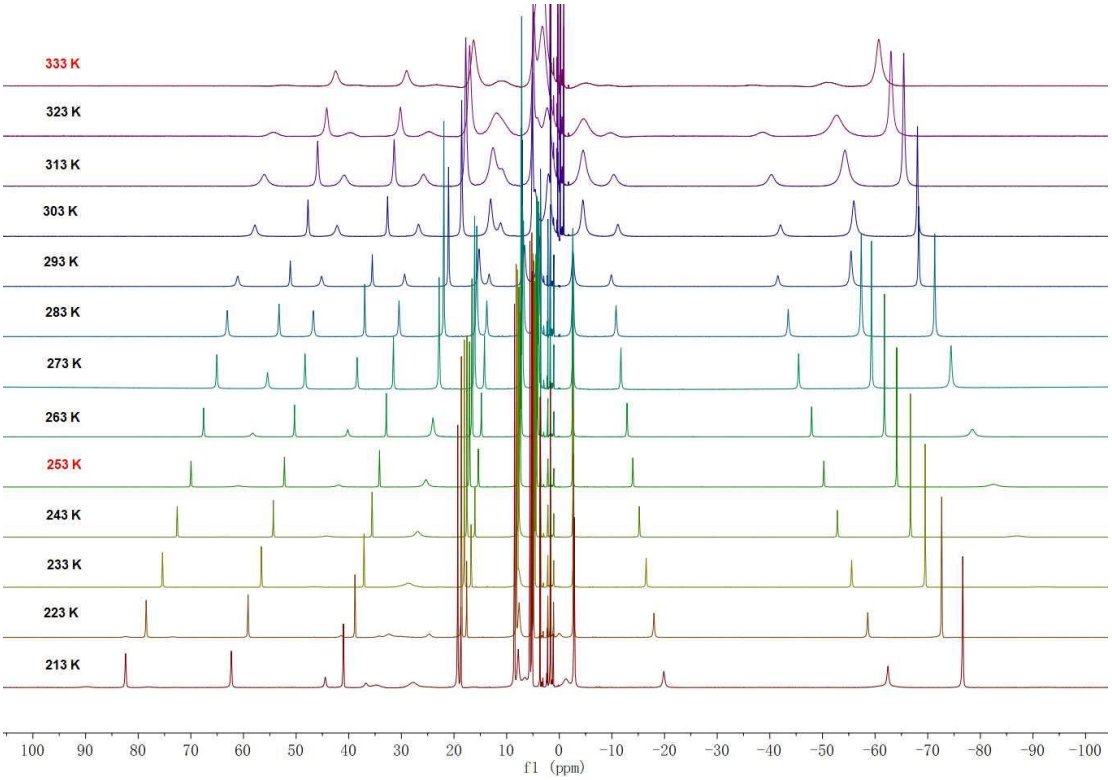


Figure S2. Variable-temperature ^{1}H NMR spectrum (from 213 K to 333 K) of complex **3** in d_8-THF.

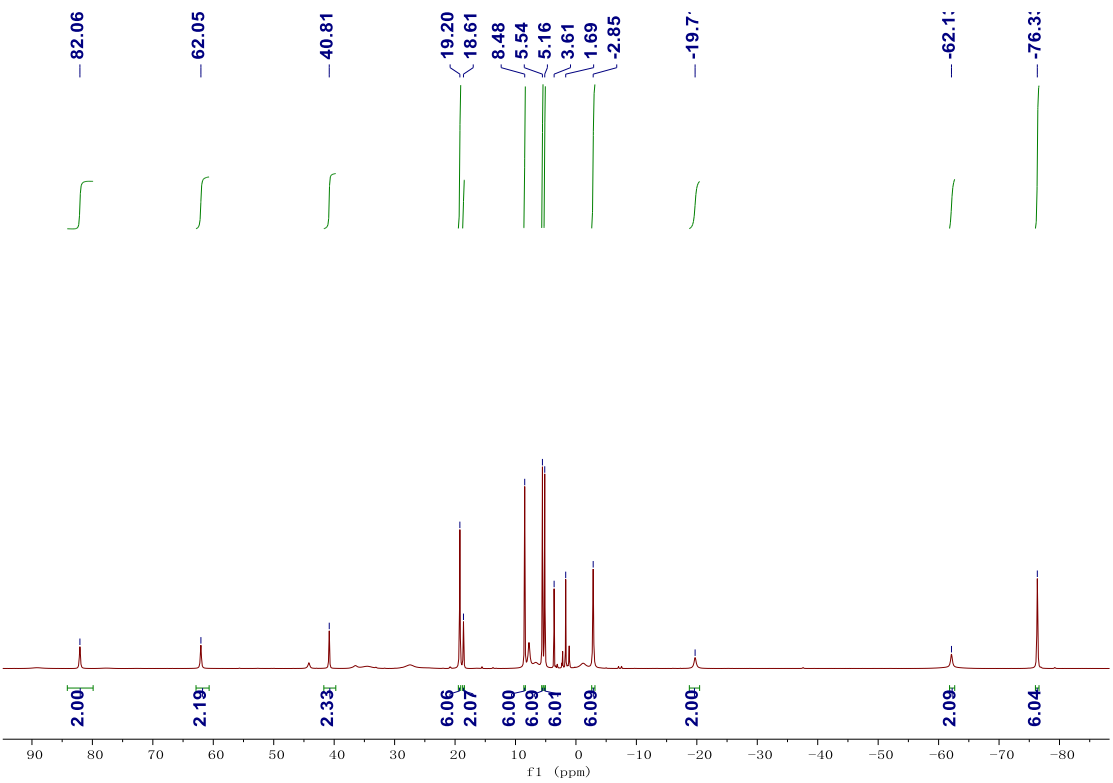


Figure S3. ^{1}H NMR spectrum of complex **3** in d_8-THF at 213 K.

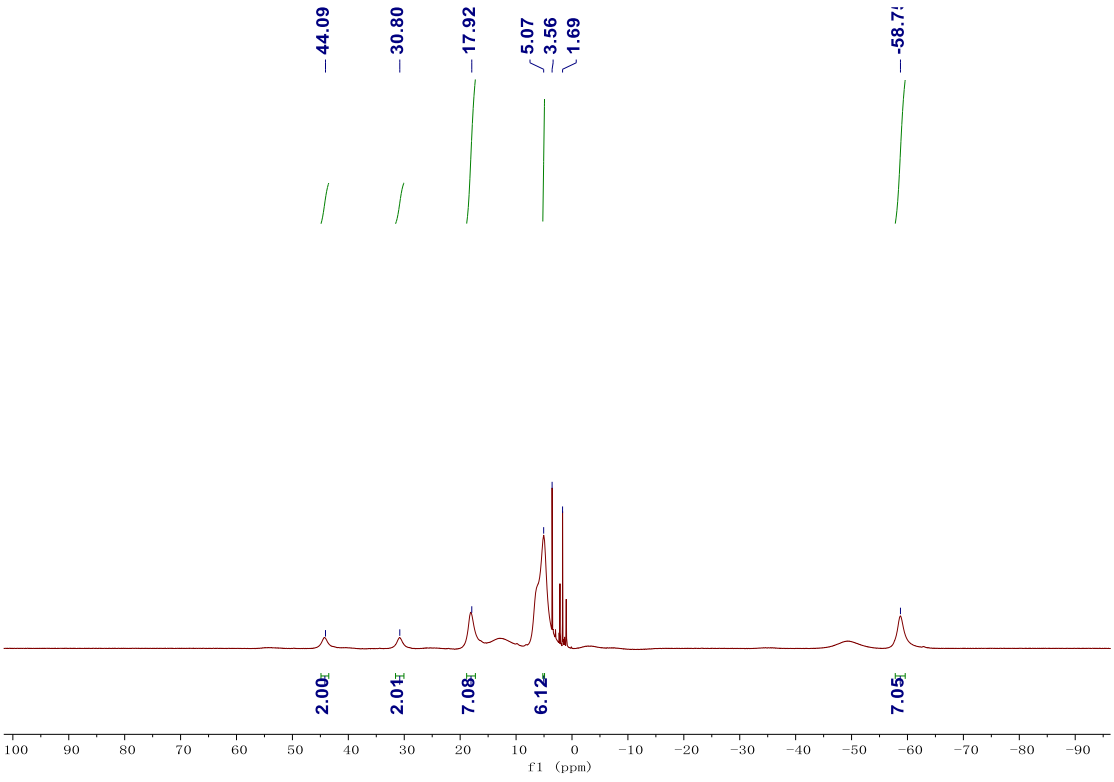


Figure S4. ^{1}H NMR spectrum of complex **2** in d_8-THF at 333 K.

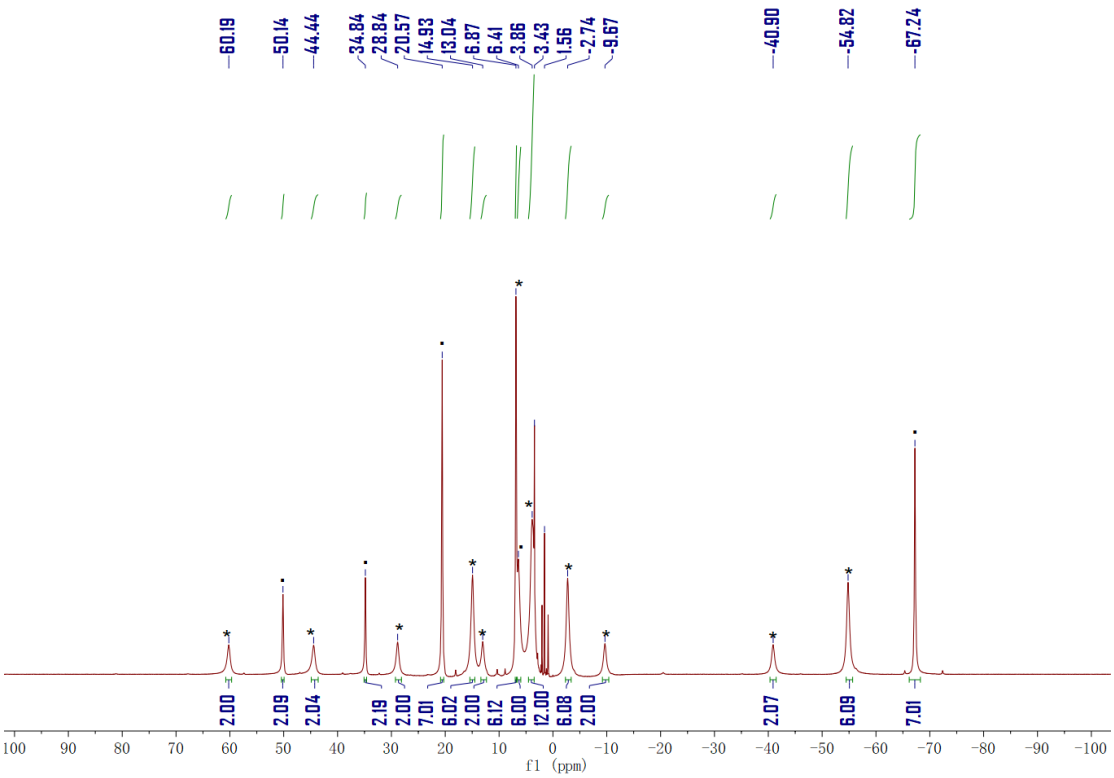


Figure S5. ^{1}H NMR spectrum (293 K) of complex **2** in d_8-THF (· complex **2**; ∗ complex **3**. The ratio of **2**:**3** = 1:1).

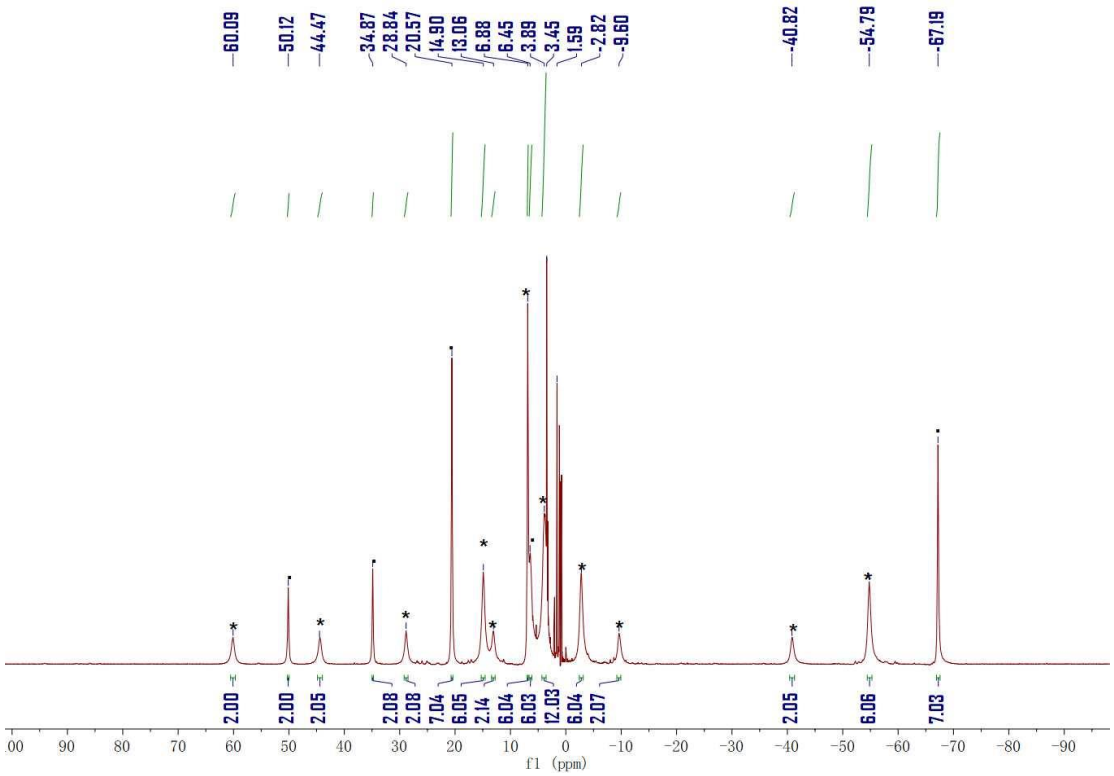


Figure S6. ^{1}H NMR spectrum (293 K) of complex **3** in d_8-THF (· complex **2**; ∗ complex **3**. The ratio of **2**:**3** = 1:1).

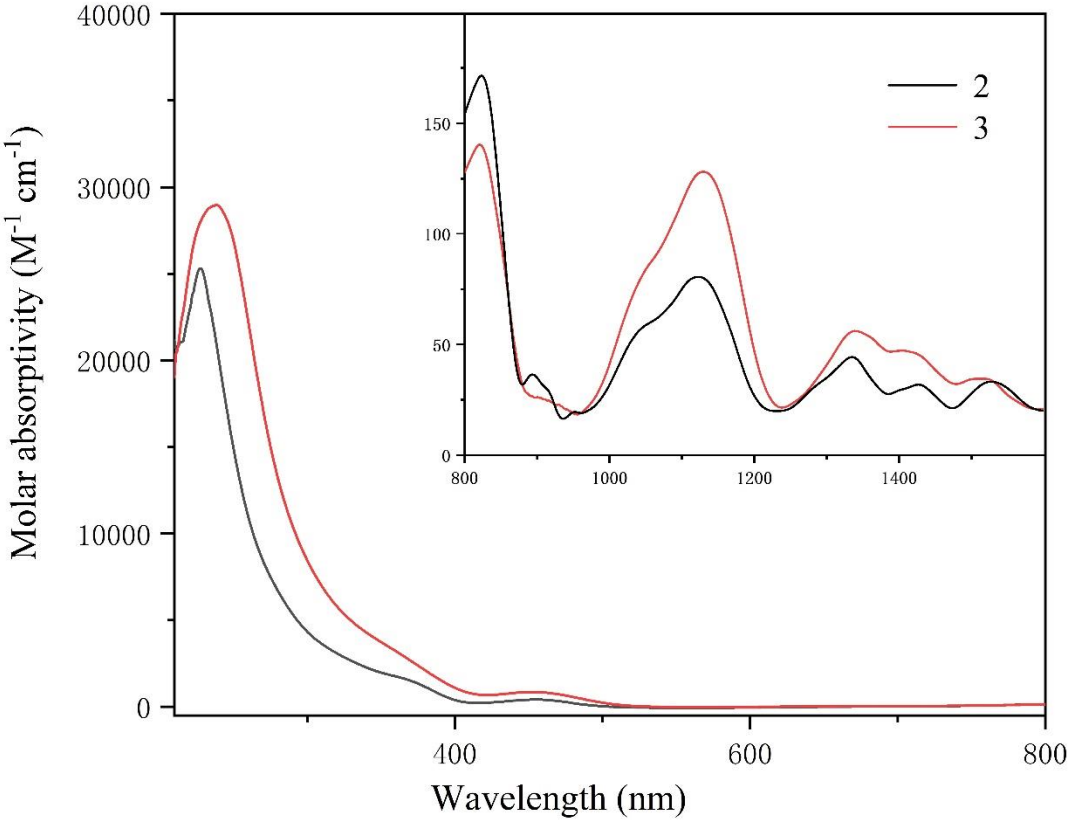


Figure. S7 UV-visible absorption spectra of **2** and **3** measured in THF at RT (inset: near infrared absorption spectra).

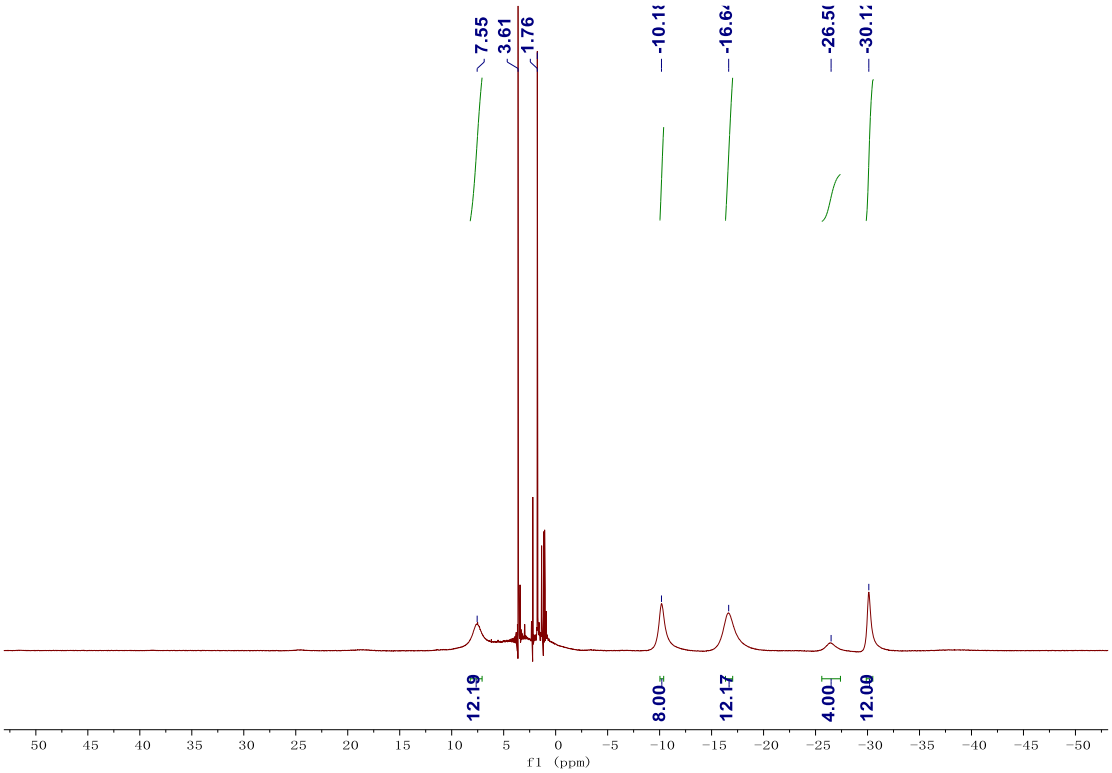


Figure S8. ^{1}H NMR spectrum of complex **4** in d_8-THF at RT.

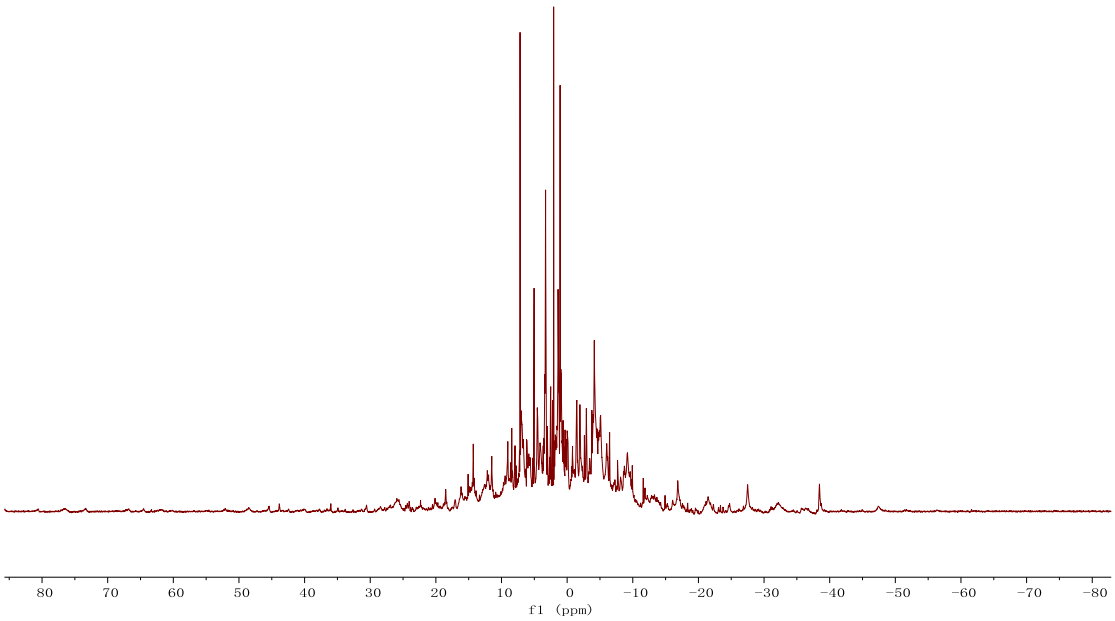


Figure S9. *In situ* ^{1}H NMR of complex **2** using a 40W UV lamp for 10 h.

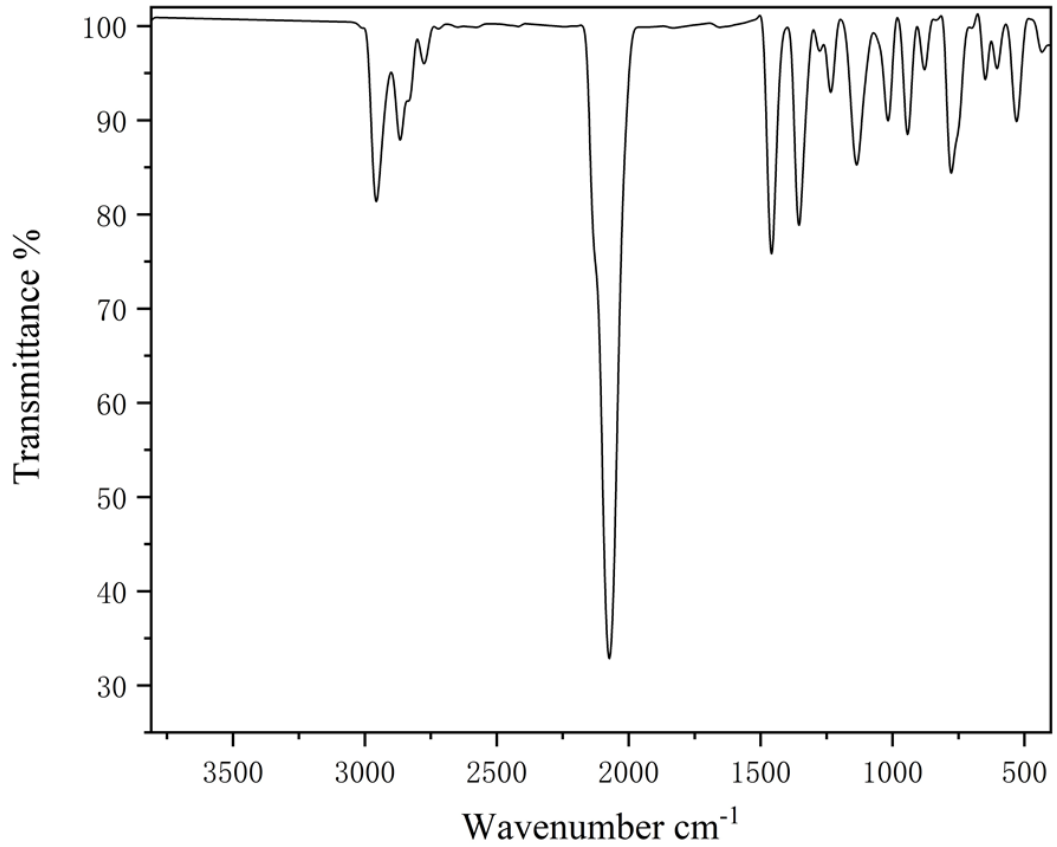


Figure S10. FT-IR spectrum of complex **2** measured as solid in a KBr pellet at RT.

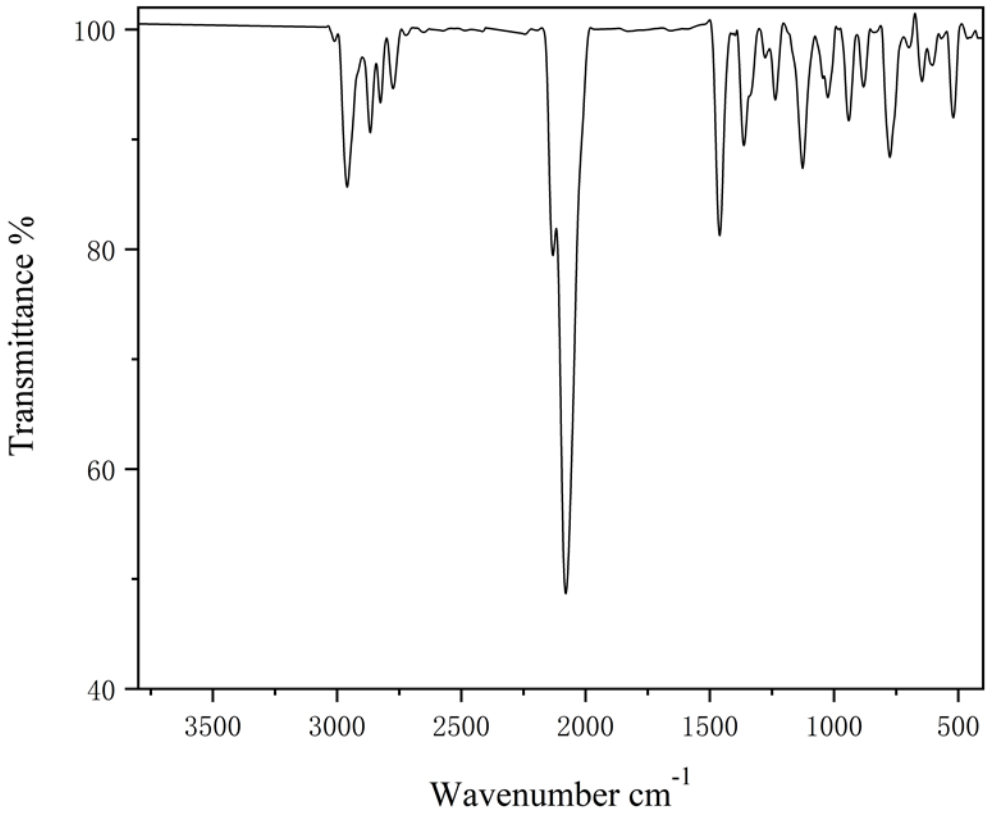


Figure S11. FT-IR spectrum of complex **3** measured as solid in a KBr pellet at RT.

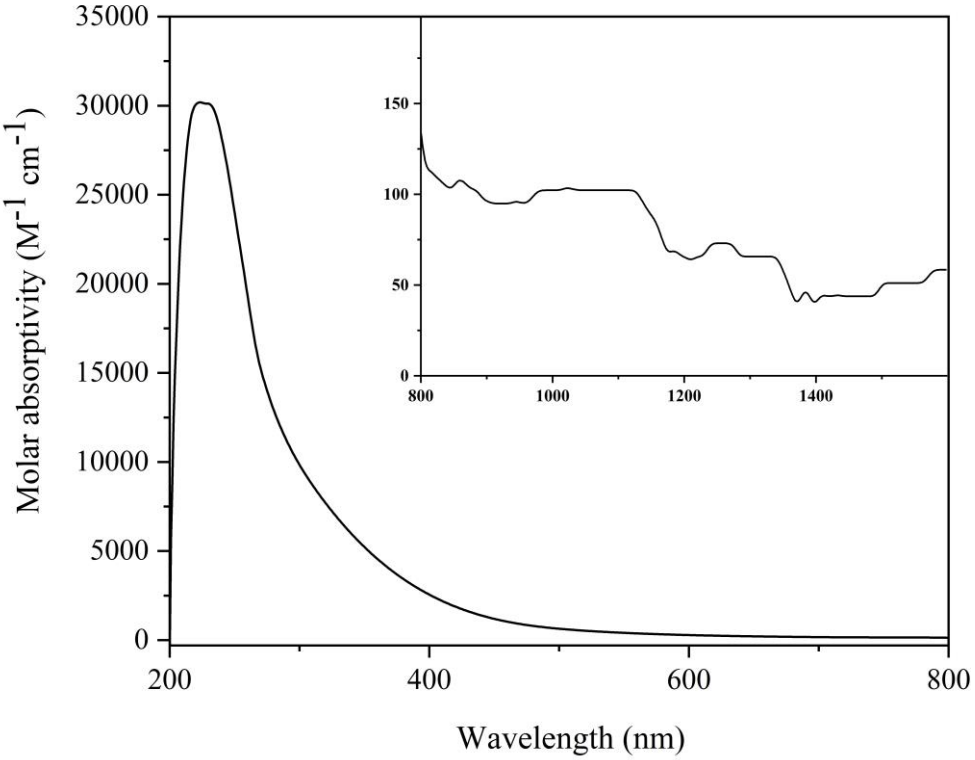


Figure S12. UV-visible absorption spectrum of complex **4** measured in THF at RT (inset: near infrared absorption spectra).

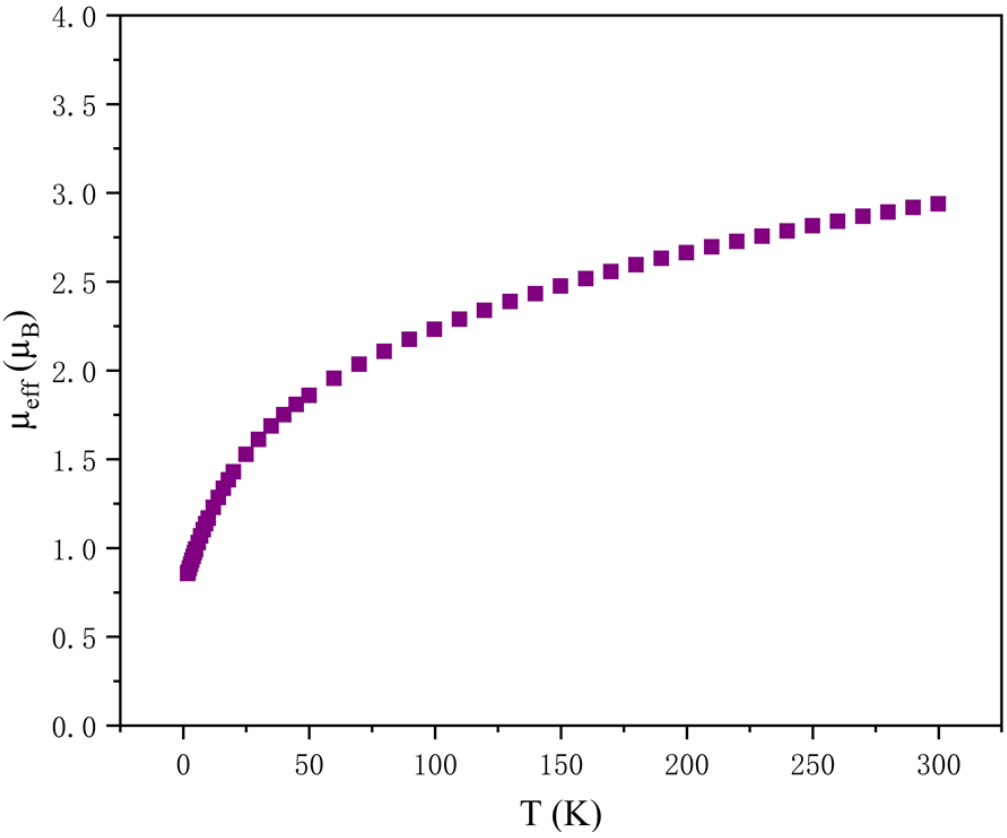
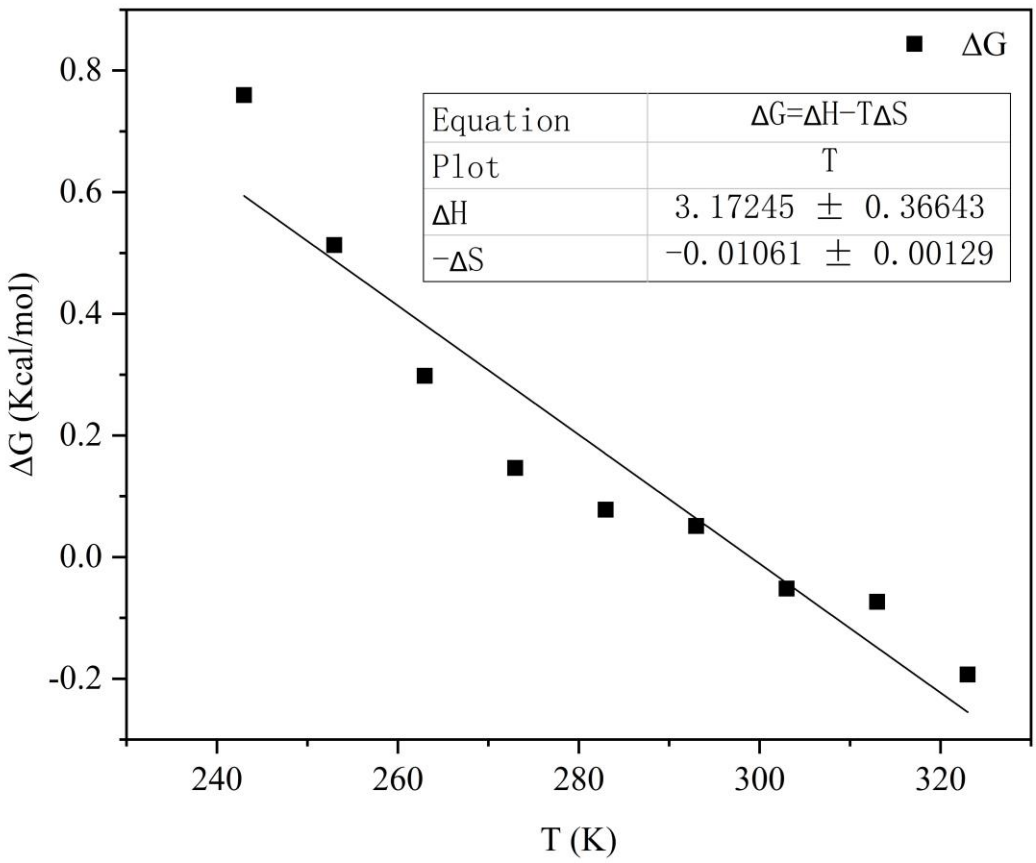


Figure S13. Variable-temperature effective magnetic moment data of complex **4** (per uranium).



dimer (**3**) $\rightleftharpoons$ 2 monomer (**2**) $\Delta G(T) = \Delta H - T\Delta S$

$$p_i = \frac{e^{-\Delta G_i/RT}}{\sum_j e^{-\Delta G_j/RT}}$$

$$p_{dimer} = \frac{e^{-\Delta G_{dimer}/RT}}{e^{-\Delta G_{dimer}/RT} + e^{-\Delta G_{2\,monomer}/RT}}$$

$$\Delta G_{dimer} = 0,\ \Delta G_{2\,monomer} = \Delta G(T)$$

$$p_{dimer} = \frac{e^{-0/RT}}{e^{-0/RT} + e^{-\Delta G(T)/RT}} = \frac{1}{1 + e^{-\Delta G(T)/RT}}$$

$$\Delta G(T) = -\mathrm{RT}\ln\left(\frac{1}{p_{dimer}} - 1\right)$$

Figure S14. The thermodynamic properties (ΔH, ΔS and ΔG) from variable temperature ^{1}H NMR spectra of complex **3**.

313K 323K 333K 343K 353K

Figure S15. A crystal of complex **3** was placed on a diffractometer and photographed at different temperature (313 K to 353 K).

40°C 50°C 60°C 70°C 80°C

Figure S16. A crystal of complex **3** was heated at incremental temperatures (40°C, 50° C, 60°C, 70°C, and 80°C) within a glovebox for 20 minutes, followed by photography at room temperature.

Complex **3** Complex **2** Complex **3**

Figure S17. The interconversion of complexes **2** and **3** in the crystal and solution states.

3. X-ray Crystallographic Analysis

The crystallographic data for complexes **2**, **3**, and **4** were collected on a Bruker D8 venture photon II detectors at 193 K or 296 K with a radiation source of Mo(Kα) (λ = 0.71073 Å) using the ω-scan technique. Multiscan or empirical absorption corrections (SADABS) were applied.[2] The structures were solved by direct methods, expanded by difference Fourier syntheses, and refined by full-matrix least squares on F^2 using the olex2.[3] All non-hydrogen atoms were refined on F^2 by full-matrix least-squares procedures with the use of anisotropic displacement parameters.[4] Hydrogen atoms were introduced at their geometric positions and refined as riding atoms. Evaluation of the CIF using the CheckCIF routine at www.checkcif.iucr.org gave no A or B alert for these complexes. Details of the data collection and refinement are given in Table S1. CCDC-2310068 (**2**), 2310070 (**3**) and 2310069 (**4**) contain the crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data-request/cif.

In addition, to corroborate the process of SCSC transformation, a crystal of complex **3** was placed on a diffractometer and X-ray diffraction data, **3-nK** (n = 313, 323, 333, 343 and 353), were collected at different temperatures (313 K, 323 K, 333 K, 343 K, and 353 K). Details of these data collection and refinement are given in Table S2. Moreover, A crystal of complex **3** was heated at incremental temperatures (40 °C, 50 °C, 60 °C, 70 °C, and 80 °C) within a glovebox for 20 minutes, followed by X-ray diffraction data collection at 193 K, **3-n °C** (n = 40, 50, 60, 70 and 80). Details of these data collection and refinement are given in Table S3.

Table S1. Crystal data and structure refinements for **2**-**4**.

Complex	**2**	**3**	**4**
Formula	$C_{20}H_{48}N_{10}P_2U$	$C_{40}H_{96}N_{20}P_4U_2$	$C_{40}H_{96}N_{10}P_4U_2$
*M*r [g/mol]	728.65	1457.30	1317.20
Temp. [K]	193.00	193.00	296.15

Crystal system	monoclinic	orthorhombic	triclinic
Space group	$P2_1/n$	$P2_12_12$	P-1
a[Å]	9.909(3)	10.5753(13)	10.769(3)
b[Å]	10.674(3)	27.797(3)	13.579(3)
c[Å]	14.833(5)	10.3786(13)	20.817(5)
α[°]	90	90	82.853(6)
β[°]	104.484(10)	90	79.684(6)
γ[°]	90	90	69.571(5)
Volume[$Å^3$]	1519.0(7)	3051.0(6)	2800.3(12)
$Z/D_{calcd.}$[g/cm^3]	2/1.593	2/1.586	2/1.562
μ[mm^{-1}]	5.474	5.451	5.925
F(000)	720.0	1440.0	1300.0
θ range/deg	4.754 - 55.008	4.12 - 54.968	3.662 - 49.998
Index ranges	$-12 \le h \le 12$ $-13 \le k \le 13$ $-19 \le l \le 19$	$-10 \le h \le 13$ $-36 \le k \le 35$ $-13 \le l \le 13$	$-12 \le h \le 12$ $-16 \le k \le 16$ $-20 \le l \le 24$
Collected data	46664	28362	15512
Unique data	3476 [R_{int} = 0.0671, R_{sigma} = 0.0259]	6999 [R_{int} = 0.1091, R_{sigma} = 0.0955]	9727 [R_{int} = 0.0523, R_{sigma} = 0.0979]
Completeness	99%	99%	99%
Data/parameters	3476/0/157	6999/0/312	9727/0/529
GOF on F^2	1.062	1.015	1.033
Final R indices [I>2 $\sigma(I)$]	R_1 = 0.0170 wR_2 = 0.0369	R_1 = 0.0467 wR_2 = 0.0860	R_1 = 0.0526 wR_2 = 0.1060
Final R indices [all data]	R_1 = 0.0256 wR_2 = 0.0388	R_1 = 0.0689 wR_2 = 0.0958	R_1 = 0.0951 wR_2 = 0.1208
Largest diff. peak/hole ($e \cdot Å^{-3}$)	0.37/-0.81	0.94/-1.30	2.39/-1.55
CCDC	2310068	2310070	2310069

Table S2. Crystal data and structure refinements for **3** at different temperature (K).

Complex	**3-313 K**	**3-323 K**	**3-333 K**	**3-343 K**	**3-353 K**
Formula	$C_{40}H_{96}N_{20}P_4U_2$	$C_{40}H_{96}N_{20}P_4U_2$	$C_{40}H_{96}N_{20}P_4U_2$	$C_{20}H_{48}N_{10}P_2U$	$C_{20}H_{48}N_{10}P_2U$
*M*r [g/mol]	1457.30	1457.30	1457.30	728.65	728.65
Temp. [K]	313.00	323.00	333.00	343.00	353.00
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	C2/c	C2/c	C2/c	C2/c	$P2_1/n$
a[Å]	25.240(4)	25.206(6)	25.279(2)	25.309(2)	10.1931(14)
b[Å]	10.392(2)	10.392(2)	10.4213(10)	10.4218(8)	10.6719(10)
c[Å]	25.465(5)	25.457(6)	25.477(3)	25.538(2)	14.9477(17)
α[°]	90	90	90	90	90
β[°]	110.915(6)	110.647(7)	110.786(3)	110.799(3)	102.736(4)
γ[°]	90	90	90	90	90
Volume[Å^3]	6239(2)	6240(2)	6274.9(11)	6297.0(9)	1586.0(3)
Z/$D_{calcd.}$[g/cm^3]	4/1.432	4/1.551	4/1.543	8/1.537	2/1.526
μ[mm^{-1}]	5.331	5.330	5.301	5.282	5.243
F(000)	2880.0	2880.0	2880.0	2880.0	720.0
θ range/deg	3.9-55.296	4.284-50.7	4.368-55.062	4.27-50.054	5.842-56.644
Index ranges	-32 ≤ h ≤ 32 -13 ≤ k ≤ 10 -32 ≤ l ≤ 33	-28 ≤ h ≤ 30 -12 ≤ k ≤ 12 -30 ≤ l ≤ 30	-32 ≤ h ≤ 32 -13 ≤ k ≤ 11 -33 ≤ l ≤ 32	-30 ≤ h ≤ 26 -12 ≤ k ≤ 12 -30 ≤ l ≤ 30	-13 ≤ h ≤ 11 -11 ≤ k ≤ 14 -19 ≤ l ≤ 12
Collected data	23910	24223	28222	18716	7496
Unique data	7215 [R_{int}=0.0883 R_{sigma}=0.0931]	5723 [R_{int}=0.0979 R_{sigma}=0.0860]	7206 [R_{int}=0.0633 R_{sigma}=0.0545]	5563 [R_{int}=0.0961 R_{sigma}=0.1070]	3940 [R_{int}=0.0714 R_{sigma}=0.0819]
Completeness	100%	100%	100%	100%	100%
Data/parameters	7215/108/370	5723/194/370	7206/141/370	5563/462/370	3940/1/157
GOF on F^2	1.026	1.008	1.012	1.055	0.906
Final R indices [I>2σ(*I*)]	R_1 = 0.0558 wR_2 = 0.0980	R_1 = 0.0530 wR_2 = 0.0910	R_1 = 0.0453 wR_2 = 0.0930	R_1 = 0.0729 wR_2 = 0.0991	R_1 = 0.0455 wR_2 = 0.1032
Final R indices [all data]	R_1 = 0.1364 wR_2 = 0.1252	R_1 = 0.1156 wR_2 = 0.1131	R_1 = 0.0924 wR_2 = 0.1133	R_1 = 0.1613 wR_2 = 0.1281	R_1 = 0.1059 wR_2 = 0.1270
Largest diff. peak/hole (e·Å^{-3})	1.50/-0.84	0.77/-0.81	1.85/-1.14	0.70/-0.91	1.23/-0.88
CCDC	2329971	2329972	2329973	2329974	2329975

Table S3. Crystal data and structure refinements for **3**.[a]

Complex	**3-40 ℃**	**3-50 ℃**	**3-60 ℃**	**3-70 ℃**	**3-80 ℃**
Formula	$C_{80}H_{192}N_{40}P_8U_4$	$C_{40}H_{96}N_{20}P_4U_2$	$C_{40}H_{96}N_{20}P_4U_2$	$C_{40}H_{96}N_{20}P_4U_2$	$C_{20}H_{48}N_{10}P_2U$
*M*r [g/mol]	2914.60	1457.30	1457.30	1457.30	728.65
Temp. [K]	193.00	193.00	193.00	193.00	193.00
Crystal system	monoclinic	orthorhombic	orthorhombic	monoclinic	monoclinic
Space group	P2/n	$P2_12_12$	$P2_12_12$	P2/n	$P2_1/n$

a[Å]	24.9458(11)	10.5761(6)	10.5757(4)	24.9421(16)	9.8845(5)
b[Å]	10.2858(5)	27.7942(16)	27.8005(13)	10.2665(7)	10.6539(6)
c[Å]	25.3172(12)	10.3688(6)	10.3708(4)	25.3542(19)	14.7678(9)
α[°]	90	90	90	90	90
β[°]	111.1580(10)	90	90	111.169(2)	104.838(2)
γ[°]	90	90	90	90	90
Volume[Å^3]	6058.2(5)	3048.0(3)	3049.1(2)	6054.3(7)	1503.31(15)
Z/$D_{calcd.}$[g/cm^3]	2/1.598	2/1.588	2/1.587	4/1.599	2/1.610
μ[mm^{-1}]	5.490	5.456	5.454	5.494	5.531
F(000)	2880.0	1440.0	1440.0	2880.0	720.0
θ range/deg	3.93-55.146	4.84-50.742	3.928-50.72	3.968-55.052	5.706-50.952
Index ranges	-32 ≤ h ≤ 32 -13 ≤ k ≤ 10 -24 ≤ l ≤ 32	-12 ≤ h ≤ 12 -33 ≤ k ≤ 33 -12 ≤ l ≤ 11	-12 ≤ h ≤ 12 -27 ≤ k ≤ 33 -12 ≤ l ≤ 12	-32 ≤ h ≤ 32 -13 ≤ k ≤ 13 -22 ≤ l ≤ 32	-11 ≤ h ≤ 11 -12 ≤ k ≤ 12 -17 ≤ l ≤ 13
Collected data	55348	24118	24195	42756	11019
Unique data	13966 [R_{int}=0.0845 R_{sigma}=0.0757]	5570 [R_{int}=0.0437 R_{sigma}=0.0426]	5586 [R_{int}=0.0604 R_{sigma}=0.0566]	13827 [R_{int}=0.0798 R_{sigma}=0.0951]	2771 [R_{int}=0.0398 R_{sigma}=0.0342]
Completeness	100%	100%	100%	100%	100%
Data/parameters	13966/31/651	5570/0/312	5586/0/311	13827/6/622	2771/0/157
GOF on F^2	1.022	0.895	0.972	1.033	1.093
Final R indices [I>2σ(I)]	R_1 = 0.0491 wR_2 = 0.0912	R_1 = 0.0185 wR_2 = 0.0397	R_1 = 0.0267 wR_2 = 0.0504	R_1 = 0.0607 wR_2 = 0.1320	R_1 = 0.0237 wR_2 = 0.0525
Final R indices [all data]	R_1 = 0.0905 wR_2 = 0.1071	R_1 = 0.0207 wR_2 = 0.0406	R_1 = 0.0324 wR_2 = 0.0525	R_1 = 0.1098 wR_2 = 0.1579	R_1 = 0.0364 wR_2 = 0.0576
Largest diff. peak/hole (e·Å^{-3})	2.03/-1.85	0.44/-0.33	0.59/-0.45	1.91/-1.84	0.98/-0.91
CCDC	2329976	2329977	2329978	2329979	2329980

[a] Complex **3** was heated at different temperatures (40 °C, 50 °C, 60 °C, 70 °C, and 80 °C) within a glovebox for 20 minutes, followed by X-ray diffraction data collection at 193 K.

4. DFT calculations

Computational details. The DFT calculations were carried out by employing hybrid functional (B3PW91)[5] along with small core pseudopotential Stuttgart basis set[6] for uranium, chlorine and phosphorus atoms (polarization functions[7] were added for phosphorus and chlorine atoms), and Pople basis set[8] (6-31G**) for the rest of the atoms. Frequency calculations were performed to locate minima for the optimized structures and for obtaining thermal corrections over the energies. To account for the solvation effects, SMD model using THF solvent has been included in the calculations.[9] All the calculations were performed using Gaussian 09 suite of programs.[10]

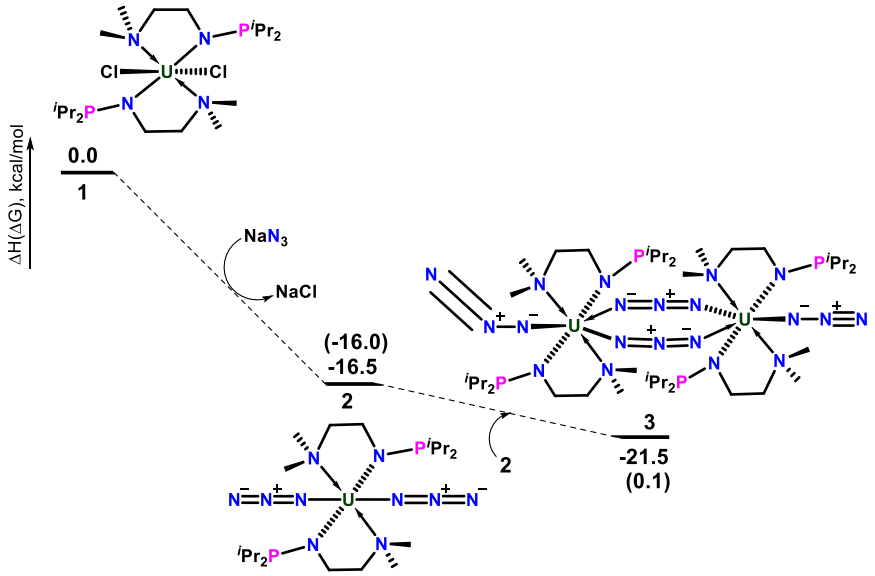


Figure S18. Computed enthalpy profile for the formation of **2** and **3** from complex **1**

Table S4. Computed Natural charges for complex **2**, s=1

Atom Label	Natural charges
U1	1.50354
N3	-1.07582
N4	-0.55263
N5	-0.52364
N6	0.25388
N19	-0.30903
N43	-1.07575
N44	-0.55281
N45	-0.52359
N46	0.25389
N59	-0.30886

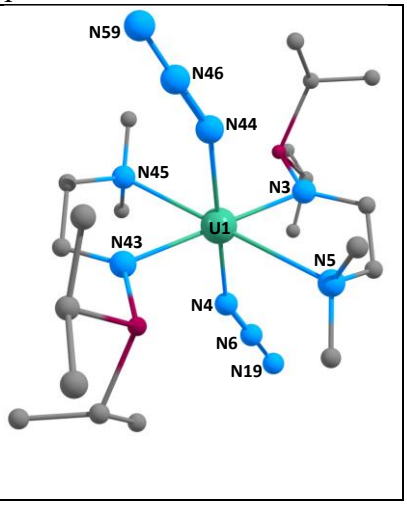


Table S5. Computed Wiberg bond index (WBI) for complex **2**, s=1

Atom Label	WBI	Atom Label	WBI	Atom Label	WBI	Atom Label	WBI
U1	0.0000	U1	0.0000	U1	0.0000	N4	0.0000
N3	0.7801	N4	0.5971	N5	0.2378	N6	1.7145
Atom Label	WBI	Atom Label	WBI	Atom Label	WBI	Atom Label	WBI
N6	0.0000	U1	0.0000	U1	0.0000	U1	0.0000
N19	2.1404	N43	0.7801	N44	0.5972	N45	0.2378
Atom Label	WBI	Atom Label	WBI				
N44	0.0000	N44	0.0000				
N46	1.7144	N59	2.1405				

Table S6. Bonding orbitals from NBO analysis for **2**, s=1

(0.97236) BD (1) U 1- N 3
(12.80%) 0.3578* U 1 s(9.52%)p 0.04(0.40%)d 4.25(40.42%) f 5.21(49.61%)g 0.00(0.04%)
(87.20%) 0.9338* N 3 s(39.81%)p 1.51(60.19%)d 0.00(0.00%)
(0.92991) BD (2) U 1- N 3
(11.86%) 0.3444* U 1 s(0.07%)p 5.54(0.41%)d99.99(49.92%) f99.99(49.58%)g 0.17(0.01%)
(88.14%) 0.9388* N 3 s(0.02%)p99.99(99.97%)d 0.66(0.01%)
(0.97604) BD (1) U 1- N 4
(9.04%) 0.3006* U 1 s(15.42%)p 0.05(0.81%)d 2.24(34.56%) f 3.19(49.19%)g 0.00(0.01%)
(90.96%) 0.9537* N 4 s(68.43%)p 0.46(31.56%)d 0.00(0.01%)
(0.95318) BD (1) U 1- N 5
(6.35%) 0.2521* U 1 s(12.66%)p 0.08(1.01%)d 2.95(37.33%) f 3.87(49.00%)g 0.00(0.00%)
(93.65%) 0.9677* N 5 s(19.94%)p 4.01(80.04%)d 0.00(0.02%)
(0.97236) BD (1) U 1- N 43
(12.80%) 0.3578* U 1 s(9.52%)p 0.04(0.40%)d 4.25(40.46%) f 5.21(49.58%)g 0.00(0.04%)
(87.20%) 0.9338* N 43 s(39.81%)p 1.51(60.18%)d 0.00(0.00%)
(0.92991) BD (2) U 1- N 43
(11.87%) 0.3445* U 1 s(0.08%)p 5.36(0.41%)d99.99(49.90%) f99.99(49.60%)g 0.16(0.01%)
(88.13%) 0.9388* N 43 s(0.02%)p99.99(99.97%)d 0.64(0.01%)
(0.97604) BD (1) U 1- N 44
(9.04%) 0.3006* U 1 s(15.41%)p 0.05(0.81%)d 2.24(34.57%) f 3.19(49.19%)g 0.00(0.02%)
(90.96%) 0.9538* N 44 s(68.43%)p 0.46(31.56%)d 0.00(0.01%)
(0.95317) BD (1) U 1- N 45

(6.35%) 0.2521* U 1 s(12.66%)p 0.08(1.01%)d 2.95(37.35%) f 3.87(48.98%)g 0.00(0.00%)
(93.65%) 0.9677* N 45 s(19.94%)p 4.01(80.04%)d 0.00(0.02%)
(0.99480) BD (1) N 4- N 6
(45.32%) 0.6732* N 4 s(31.53%)p 2.17(68.28%)d 0.01(0.19%)
(54.68%) 0.7395* N 6 s(50.30%)p 0.99(49.62%)d 0.00(0.08%)
(0.99648) BD (1) N 6- N 19
(56.43%) 0.7512* N 6 s(49.32%)p 1.03(50.60%)d 0.00(0.08%)
(43.57%) 0.6601* N 19 s(32.09%)p 2.11(67.58%)d 0.01(0.33%)
(0.99419) BD (2) N 6- N 19
(50.54%) 0.7109* N 6 s(0.17%)p99.99(99.66%)d 0.99(0.17%)
(49.46%) 0.7033* N 19 s(0.16%)p99.99(99.46%)d 2.41(0.38%)
(0.99332) BD (3) N 6- N 19
(50.77%) 0.7125* N 6 s(0.03%)p99.99(99.80%)d 5.06(0.17%)
(49.23%) 0.7017* N 19 s(0.03%)p99.99(99.59%)d10.93(0.38%)
(0.99480) BD (1) N 44- N 46
(45.32%) 0.6732* N 44 s(31.53%)p 2.17(68.29%)d 0.01(0.19%)
(54.68%) 0.7395* N 46 s(50.30%)p 0.99(49.62%)d 0.00(0.08%)
(0.99648) BD (1) N 46- N 59
(56.43%) 0.7512* N 46 s(49.32%)p 1.03(50.60%)d 0.00(0.08%)
(43.57%) 0.6601* N 59 s(32.09%)p 2.11(67.58%)d 0.01(0.33%)
(0.99420) BD (2) N 46- N 59
(50.54%) 0.7109* N 46 s(0.17%)p99.99(99.66%)d 0.99(0.17%)
(49.46%) 0.7033* N 59 s(0.16%)p99.99(99.46%)d 2.43(0.38%)
(0.99332) BD (3) N 46- N 59
(50.77%) 0.7125* N 46 s(0.03%)p99.99(99.80%)d 5.11(0.17%)
(49.23%) 0.7017* N 59 s(0.03%)p99.99(99.59%)d11.06(0.38%)

Table S7. Second order perturbation analysis for **2**, s=1

Donor NBO	Acceptor NBO	E(2) kcal/mol
(0.71376) LP (1) N 4 s(0.07%)p99.99(99.81%)d 1.62(0.11%)	(0.07444) LV (1) U 1 s(0.90%)p 0.00(0.00%)d99.99(99.08%)f 0.00(0.00%)g 0.02(0.02%)	6.33
(0.71376) LP (1) N 4 s(0.07%)p99.99(99.81%)d 1.62(0.11%)	(0.23979) BD*(2) N 6- N 19 (49.46%) 0.7033* N 6 s(0.17%)p99.99(99.66%)d 0.99(0.17%) (50.54%) -0.7109* N 19 s(0.16%)p99.99(99.46%)d 2.41(0.38%)	59.11
(0.71376) LP (1) N 4 s(0.07%)p99.99(99.81%)d 1.62(0.11%)	(0.23731) BD*(3) N 6- N 19 (49.23%) 0.7017* N 6 s(0.03%)p99.99(99.80%)d 5.06(0.17%) (50.77%) -0.7125* N 19 s(0.03%)p99.99(99.59%)d10.93(0.38%)	20.22

(0.70328) LP (2) N 4 s(0.01%)p99.99(99.86%)d 10.29(0.12%)	(0.07444) LV (1) U 1 s(0.90%)p 0.00(0.00%)d99.99(99.08%)f 0.00(0.00%)g 0.02(0.02%)	7.15
(0.70328) LP (2) N 4 s(0.01%)p99.99(99.86%)d 10.29(0.12%)	(0.23979) BD*(2) N 6- N 19 (49.46%) 0.7033* N 6 s(0.17%)p99.99(99.66%)d 0.99(0.17%) (50.54%) -0.7109* N 19 s(0.16%)p99.99(99.46%)d 2.41(0.38%)	21.91
(0.70328) LP (2) N 4 s(0.01%)p99.99(99.86%)d 10.29(0.12%)	(0.23731) BD*(3) N 6- N 19 (49.23%) 0.7017* N 6 s(0.03%)p99.99(99.80%)d 5.06(0.17%) (50.77%) -0.7125* N 19 s(0.03%)p99.99(99.59%)d10.93(0.38 %)	65.49
(0.71377) LP (1) N 44 s(0.07%)p99.99(99.81%)d 1.62(0.11%)	(0.07444) LV (1) U 1 s(0.90%)p 0.00(0.00%)d99.99(99.08%)f 0.00(0.00%)g 0.02(0.02%)	6.30
(0.71377) LP (1) N 44 s(0.07%)p99.99(99.81%)d 1.62(0.11%)	(0.23973) BD*(2) N 46- N 59 (49.46%) 0.7033* N 46 s(0.17%)p99.99(99.66%)d 0.99(0.17%) (50.54%) -0.7109* N 59 s(0.16%)p99.99(99.46%)d 2.43(0.38%)	59.21
(0.71377) LP (1) N 44 s(0.07%)p99.99(99.81%)d 1.62(0.11%)	(0.23728) BD*(3) N 46- N 59 (49.23%) 0.7017* N 46 s(0.03%)p99.99(99.80%)d 5.11(0.17%) (50.77%) -0.7125* N 59 s(0.03%)p99.99(99.59%)d11.06(0.38 %)	20.12
(0.70333) LP (2) N 44 s(0.01%)p99.99(99.86%)d 10.26(0.12%)	(0.07444) LV (1) U 1 s(0.90%)p 0.00(0.00%)d99.99(99.08%)f 0.00(0.00%)g 0.02(0.02%)	7.11
(0.70333) LP (2) N 44 s(0.01%)p99.99(99.86%)d 10.26(0.12%)	(0.23973) BD*(2) N 46- N 59 (49.46%) 0.7033* N 46 s(0.17%)p99.99(99.66%)d 0.99(0.17%) (50.54%) -0.7109* N 59 s(0.16%)p99.99(99.46%)d 2.43(0.38%)	21.79
(0.70333) LP (2) N 44 s(0.01%)p99.99(99.86%)d 10.26(0.12%)	(0.23728) BD*(3) N 46- N 59 (49.23%) 0.7017* N 46 s(0.03%)p99.99(99.80%)d 5.11(0.17%) (50.77%) -0.7125* N 59 s(0.03%)p99.99(99.59%)d11.06(0.38 %)	65.59
(0.98662) LP (1) N 59 s(68.13%)p 0.47(31.83%)d 0.00(0.04%)	(0.01448) BD*(1) N 44- N 46 (54.68%) 0.7395* N 44 s(31.53%)p 2.17(68.29%)d 0.01(0.19%) (45.32%) -0.6732* N 46 s(50.30%)p 0.99(49.62%)d 0.00(0.08%)	8.77

(0.97604) BD (1) U 1- N 4 (9.04%) 0.3006* U 1 s(15.42%)p 0.05(0.81%)d 2.24(34.56%) f 3.19(49.19%)g 0.00(0.01%) (90.96%) 0.9537* N 4 s(68.43%)p 0.46(31.56%)d 0.00(0.01%)	(0.00967) BD*(1) N 6- N 19 (43.57%) 0.6601* N 6 s(49.32%)p 1.03(50.60%)d 0.00(0.08%) (56.43%) -0.7512* N 19 s(32.09%)p 2.11(67.58%)d 0.01(0.33%)	7.90
(0.97604) BD (1) U 1- N 44 (9.04%) 0.3006* U 1 s(15.41%)p 0.05(0.81%)d 2.24(34.57%) f 3.19(49.19%)g 0.00(0.02%) (90.96%) 0.9538* N 44 s(68.43%)p 0.46(31.56%)d 0.00(0.01%)	(0.00966) BD*(1) N 46- N 59 (43.57%) 0.6601* N 46 s(49.32%)p 1.03(50.60%)d 0.00(0.08%) (56.43%) -0.7512* N 59 s(32.09%)p 2.11(67.58%)d 0.01(0.33%)	7.90

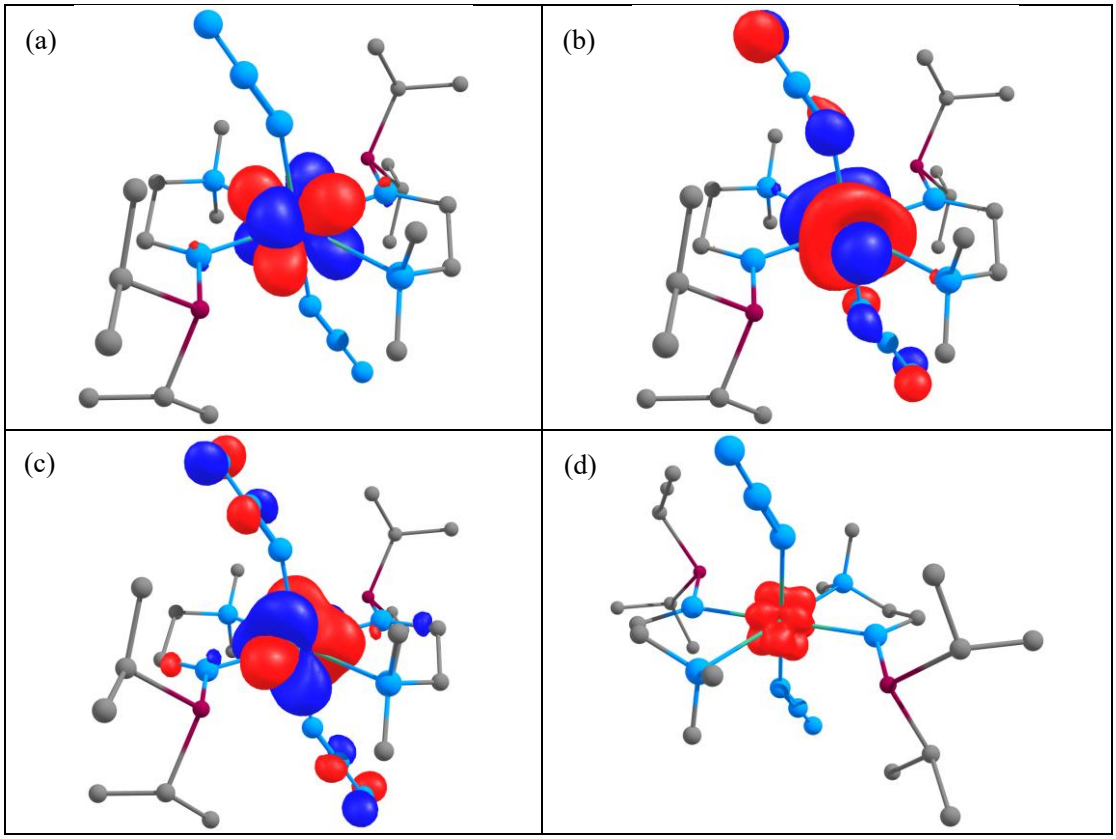


Figure S19. Computed MO's for **2**, s=1. (a)HOMO-1 (b)HOMO (c)LUMO (d)spin density plot (s=1)

Table S8. Spin energetics for **3**

Spin states	ΔH (kcal/mol)
s=2	0.1
s=1	10.5
s=0 (open-shell)	0.0

Table S9. Computed Natural charges for complex **3**, s=2

Atom Label	Natural charges
U1	1.27712
N4	-1.05282
N5	-1.05203
N6	-0.50159
N7	-0.50653
N8	0.31508
N9	-0.52073
N10	0.31064
N11	-0.38291
N14	-0.38924
N37	0.25783
N74	-0.31298
N83	-0.37557
N84	-0.38071
U85	1.27400
N88	-1.05414
N89	-1.05316
N90	-0.50094
N91	-0.50823
N92	-0.52773
N117	0.25742
N154	-0.31149

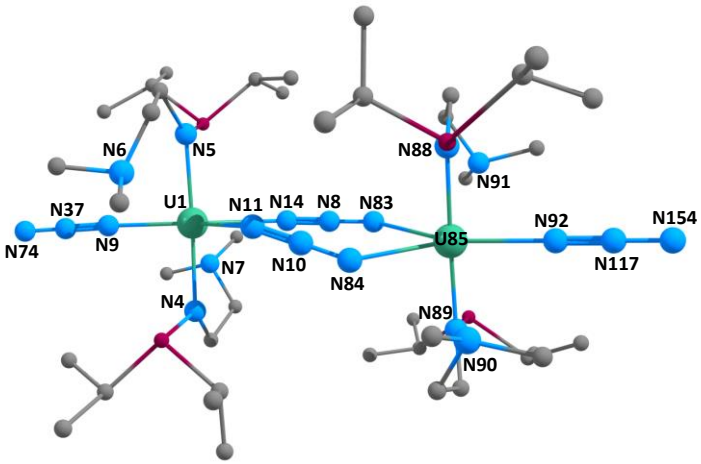


Table S10. Computed Wiberg bond index (WBI) for complex **3**, s=2

Atom Label	WBI	Atom Label	WBI	Atom Label	WBI	Atom Label	WBI
U1	0.0000	U1	0.0000	U1	0.0000	U1	0.0000
N4	0.8285	N5	0.8199	N6	0.2119	N7	0.2283
Atom Label	WBI	Atom Label	WBI	Atom Label	WBI	Atom Label	WBI
U1	0.0000	U1	0.0000	U1	0.0000	N10	0.0000
N9	0.6387	N11	0.4324	N14	0.4361	N11	1.9152
Atom Label	WBI	Atom Label	WBI	Atom Label	WBI	Atom Label	WBI
N10	0.0000	U85	0.0000	U85	0.0000	U85	0.0000
N84	1.9184	N83	0.4238	N84	0.4310	N88	0.8321
Atom Label	WBI	Atom Label	WBI	Atom Label	WBI	Atom Label	WBI
U85	0.0000	U85	0.0000	U85	0.0000	U85	0.0000
N89	0.8223	N90	0.2175	N91	0.2293	N92	0.6340
Atom Label	WBI	Atom Label	WBI	Atom Label	WBI	Atom Label	WBI

N8	0.0000	N8	0.0000	N37	0.0000	N37	0.0000
N14	1.9088	N83	1.9294	N9	1.7195	N74	2.1342
Atom Label	WBI	Atom Label	WBI				
N117	0.0000	N117	0.0000				
N92	1.7186	N154	2.1354				

Table S11. Bonding orbitals from NBO analysis for **3**, s=2

(0.97221) BD (1) U 1- N 4
(13.26%) 0.3641* U 1 s(10.34%)p 0.05(0.47%)d 3.72(38.53%) f 4.89(50.62%)g 0.00(0.05%)
(86.74%) 0.9314* N 4 s(40.93%)p 1.44(59.07%)d 0.00(0.00%)
(0.93362) BD (2) U 1- N 4
(12.81%) 0.3579* U 1 s(0.05%)p29.70(1.62%)d99.99(49.95%) f99.99(48.33%)g 0.81(0.04%)
(87.19%) 0.9338* N 4 s(0.03%)p99.99(99.97%)d 0.35(0.01%)
(0.97244) BD (1) U 1- N 5
(13.17%) 0.3629* U 1 s(10.74%)p 0.05(0.51%)d 3.73(40.02%) f 4.53(48.69%)g 0.00(0.05%)
(86.83%) 0.9318* N 5 s(41.37%)p 1.42(58.62%)d 0.00(0.01%)
(0.93035) BD (2) U 1- N 5
(12.60%) 0.3549* U 1 s(0.03%)p43.04(1.48%)d99.99(51.21%) f99.99(47.23%)g 1.46(0.05%)
(87.40%) 0.9349* N 5 s(0.03%)p99.99(99.95%)d 0.40(0.01%)
(0.94334) BD (1) U 1- N 7
(5.49%) 0.2344* U 1 s(8.92%)p 0.48(4.30%)d 4.01(35.76%) f 5.72(50.98%)g 0.00(0.04%)
(94.51%) 0.9721* N 7 s(19.49%)p 4.13(80.49%)d 0.00(0.02%)
(0.96422) BD (1) U 1- N 9
(8.93%) 0.2989* U 1 s(14.69%)p 0.26(3.87%)d 3.01(44.21%) f 2.52(37.01%)g 0.02(0.22%)
(91.07%) 0.9543* N 9 s(66.80%)p 0.50(33.20%)d 0.00(0.00%)
(0.96370) BD (1) U 1- N 11
(7.85%) 0.2801* U 1 s(11.85%)p 0.33(3.89%)d 4.94(58.51%) f 2.16(25.61%)g 0.01(0.13%)
(92.15%) 0.9600* N 11 s(68.38%)p 0.46(31.60%)d 0.00(0.02%)
(0.96367) BD (1) U 1- N 14
(7.55%) 0.2748* U 1 s(11.48%)p 0.42(4.78%)d 4.30(49.37%) f 2.98(34.22%)g 0.01(0.16%)
(92.45%) 0.9615* N 14 s(68.22%)p 0.47(31.77%)d 0.00(0.02%)
(0.95944) BD (1) N 83- U 85
(92.21%) 0.9603* N 83 s(66.88%)p 0.50(33.11%)d 0.00(0.01%)
(7.79%) 0.2791* U 85 s(12.44%)p 0.39(4.83%)d 3.92(48.79%) f 2.71(33.78%)g 0.01(0.15%)
(0.96058) BD (1) N 84- U 85
(91.99%) 0.9591* N 84 s(66.90%)p 0.49(33.09%)d 0.00(0.02%)

(8.01%) 0.2831* U 85 s(12.52%)p 0.31(3.84%)d 4.81(60.24%) f 1.86(23.27%)g 0.01(0.13%)
(0.97055) BD (1) U 85- N 88
(13.59%) 0.3687* U 85 s(10.34%)p 0.05(0.48%)d 3.73(38.56%) f 4.89(50.57%)g 0.01(0.05%)
(86.41%) 0.9296* N 88 s(40.57%)p 1.46(59.42%)d 0.00(0.01%)
(0.93427) BD (2) U 85- N 88
(12.44%) 0.3527* U 85 s(0.09%)p18.61(1.64%)d99.99(49.46%) f99.99(48.77%)g 0.56(0.05%)
(87.56%) 0.9357* N 88 s(0.04%)p99.99(99.95%)d 0.20(0.01%)
(0.97087) BD (1) U 85- N 89
(13.49%) 0.3673* U 85 s(10.69%)p 0.05(0.53%)d 3.75(40.03%) f 4.56(48.70%)g 0.00(0.05%)
(86.51%) 0.9301* N 89 s(40.97%)p 1.44(59.03%)d 0.00(0.01%)
(0.93054) BD (2) U 85- N 89
(12.18%) 0.3489* U 85 s(0.04%)p41.40(1.59%)d99.99(51.08%) f99.99(47.24%)g 1.41(0.05%)
(87.82%) 0.9371* N 89 s(0.04%)p99.99(99.95%)d 0.33(0.01%)
(0.94244) BD (1) U 85- N 90
(5.27%) 0.2295* U 85 s(8.64%)p 0.55(4.74%)d 4.55(39.36%) f 5.46(47.22%)g 0.01(0.05%)
(94.73%) 0.9733* N 90 s(18.20%)p 4.49(81.77%)d 0.00(0.03%)
(0.94384) BD (1) U 85- N 91
(5.55%) 0.2356* U 85 s(9.05%)p 0.44(4.00%)d 4.34(39.33%) f 5.25(47.57%)g 0.00(0.04%)
(94.45%) 0.9719* N 91 s(19.34%)p 4.17(80.64%)d 0.00(0.02%)
(0.96586) BD (1) U 85- N 92
(8.08%) 0.2842* U 85 s(15.81%)p 0.25(3.99%)d 2.93(46.30%) f 2.13(33.66%)g 0.02(0.24%)
(91.92%) 0.9588* N 92 s(67.32%)p 0.49(32.68%)d 0.00(0.00%)

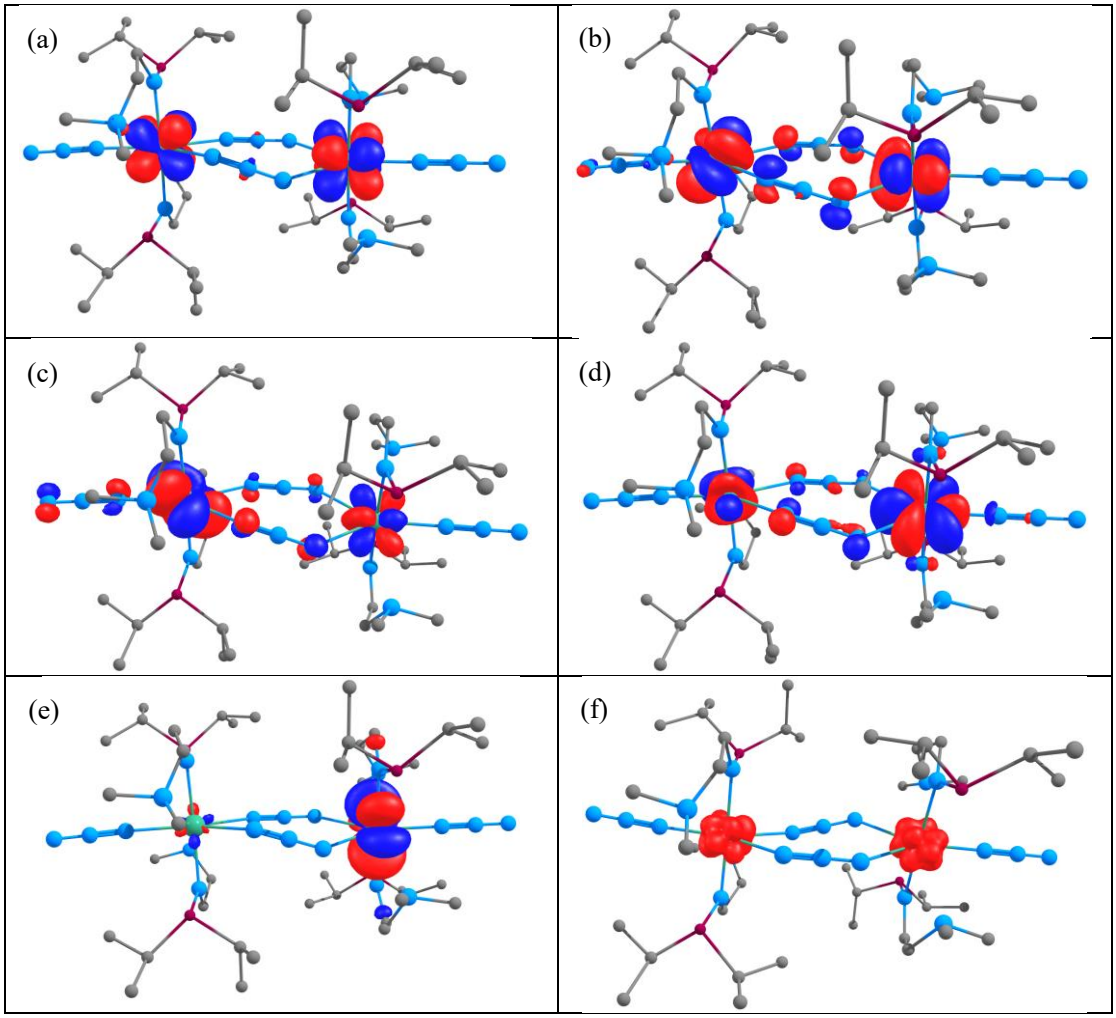


Figure S20. DFT computed MO's for **3**, s=2. (a) HOMO-3 (b) HOMO-2 (c) HOMO-1 (d) HOMO (e) LUMO (f) spin density plot

Table S12. Computed spin states for **4**

Spin states	ΔH (ΔG), kcal/mol
s=1	0.1 (0.0)
s=0	30.7 (33.7)
s=0 (open shell)	0.0 (0.2)

Table S13. Computed Natural charges for complex **4**, s=1

Atom Label	Natural charges
U1	1.54337
U2	1.72280
N7	-0.98627
N8	-0.50927
N9	-0.98637
N10	-0.51030
N15	-1.11918
N16	-0.49664
N17	-1.09286
N18	-1.11909
N19	-0.49857
N20	-1.08886

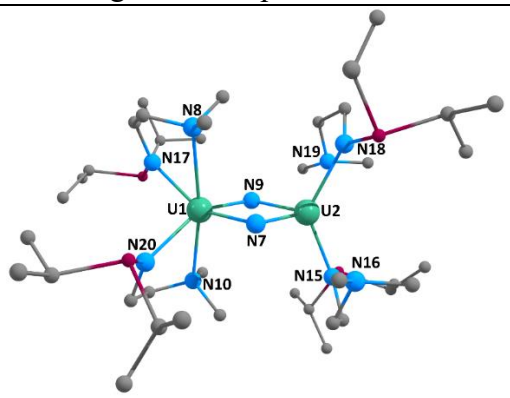


Table S14. Computed Wiberg bond index (WBI) for complex **4**, s=1

Atom Label	WBI	Atom Label	WBI	Atom Label	WBI	Atom Label	WBI
U1	0.0000	U1	0.0000	U1	0.0000	U1	0.0000
N7	1.4338	N9	1.3785	N8	0.2607	N10	0.2616
Atom Label	WBI	Atom Label	WBI	Atom Label	WBI	Atom Label	WBI
U1	0.0000	U1	0.0000	U2	0.0000	U2	0.0000
N17	0.6698	N20	0.6787	N7	1.3690	N9	1.4292
Atom Label	WBI	Atom Label	WBI	Atom Label	WBI	Atom Label	WBI
U2	0.0000	U2	0.0000	U2	0.0000	U2	0.0000
N15	0.6358	N16	0.2076	N18	0.6321	N19	0.2167
Atom Label	WBI	Atom Label	WBI				
U1	0.0000	N7	0.0000				
U2	0.5015	N9	0.0276				

Table S15. Bonding orbitals from NBO analysis for **4**, s=1

(0.96184) BD (1) U 1- N 7
(18.30%) 0.4278* U 1 s(7.66%)p 0.04(0.30%)d 6.11(46.75%) f 5.91(45.26%)g 0.00(0.04%)
(81.70%) 0.9039* N 7 s(48.70%)p 1.05(51.21%)d 0.00(0.09%)
(0.95498) BD (1) U 1- N 8
(8.06%) 0.2839* U 1 s(13.01%)p 0.06(0.72%)d 3.29(42.76%) f 3.34(43.50%)g 0.00(0.01%)
(91.94%) 0.9588* N 8 s(21.07%)p 3.75(78.92%)d 0.00(0.01%)
(0.96154) BD (1) U 1- N 9
(17.95%) 0.4237* U 1 s(8.38%)p 0.04(0.30%)d 5.82(48.76%) f 5.08(42.53%)g 0.00(0.04%)
(82.05%) 0.9058* N 9 s(48.64%)p 1.05(51.27%)d 0.00(0.09%)
(0.95529) BD (1) U 1- N 10
(8.09%) 0.2845* U 1 s(12.07%)p 0.06(0.72%)d 3.59(43.29%) f 3.64(43.90%)g 0.00(0.01%)

(91.91%) 0.9587* N 10 s(21.19%)p 3.72(78.80%)d 0.00(0.01%)
(0.97032) BD (1) U 1- N 17
(12.33%) 0.3512* U 1 s(11.60%)p 0.05(0.59%)d 3.91(45.36%) f 3.66(42.41%)g 0.00(0.03%)
(87.67%) 0.9363* N 17 s(40.51%)p 1.47(59.49%)d 0.00(0.00%)
(0.91607) BD (2) U 1- N 17
(8.23%) 0.2870* U 1 s(0.02%)p30.25(0.69%)d99.99(47.19%) f99.99(52.05%)g 1.90(0.04%)
(91.77%) 0.9579* N 17 s(0.00%)p 1.00(99.98%)d 0.00(0.02%)
(0.97125) BD (1) U 1- N 20
(12.45%) 0.3529* U 1 s(11.08%)p 0.05(0.53%)d 3.98(44.07%) f 4.00(44.28%)g 0.00(0.03%)
(87.55%) 0.9357* N 20 s(40.46%)p 1.47(59.53%)d 0.00(0.01%)
(0.91845) BD (2) U 1- N 20
(8.39%) 0.2897* U 1 s(0.28%)p 2.66(0.76%)d99.99(46.79%) f99.99(52.12%)g 0.16(0.04%)
(91.61%) 0.9571* N 20 s(0.02%)p99.99(99.97%)d 0.83(0.02%)
(0.95522) BD (1) U 2- N 7
(18.21%) 0.4268* U 2 s(6.81%)p 0.06(0.41%)d 6.61(44.99%) f 7.01(47.75%)g 0.01(0.04%)
(81.79%) 0.9044* N 7 s(47.75%)p 1.09(52.15%)d 0.00(0.10%)
(0.95695) BD (1) U 2- N 9
(18.36%) 0.4285* U 2 s(6.62%)p 0.06(0.41%)d 6.72(44.46%) f 7.33(48.48%)g 0.01(0.04%)
(81.64%) 0.9036* N 9 s(47.08%)p 1.12(52.82%)d 0.00(0.10%)
(0.97186) BD (1) U 2- N 15
(9.25%) 0.3042* U 2 s(15.43%)p 0.05(0.73%)d 3.67(56.66%) f 1.76(27.14%)g 0.00(0.04%)
(90.75%) 0.9526* N 15 s(41.33%)p 1.42(58.66%)d 0.00(0.00%)
(0.92170) BD (2) U 2- N 15
(9.56%) 0.3093* U 2 s(0.25%)p 0.94(0.23%)d99.99(57.65%) f99.99(41.85%)g 0.10(0.02%)
(90.44%) 0.9510* N 15 s(0.07%)p99.99(99.92%)d 0.20(0.01%)
(0.94704) BD (1) U 2- N 16
(5.75%) 0.2399* U 2 s(12.09%)p 0.07(0.81%)d 3.20(38.66%) f 4.01(48.44%)g 0.00(0.01%)
(94.25%) 0.9708* N 16 s(16.54%)p 5.04(83.43%)d 0.00(0.03%)
(0.97191) BD (1) U 2- N 18
(9.55%) 0.3091* U 2 s(15.21%)p 0.05(0.69%)d 3.61(54.97%) f 1.91(29.10%)g 0.00(0.03%)
(90.45%) 0.9510* N 18 s(41.10%)p 1.43(58.90%)d 0.00(0.00%)
(0.92110) BD (2) U 2- N 18
(9.35%) 0.3058* U 2 s(0.26%)p 0.94(0.25%)d99.99(58.32%) f99.99(41.15%)g 0.10(0.02%)

(90.65%) 0.9521* N 18 s(0.09%)p99.99(99.89%)d 0.16(0.01%)
(0.94758) BD (1) U 2- N 19
(6.04%) 0.2458* U 2 s(12.61%)p 0.06(0.75%)d 3.07(38.70%) f 3.80(47.93%)g 0.00(0.01%)
(93.96%) 0.9693* N 19 s(16.93%)p 4.91(83.05%)d 0.00(0.03%)

Table S16. Second order perturbation analysis for **4**, s=1

Donor NBO	Acceptor NBO	E(2) kcal/mol
(0.67586) LP (1) N 7 s(2.60%)p37.39(97.26%)d 0.05(0.14%)	(0.16017) LV (1) U 1 s(9.44%)p 0.02(0.15%)d 3.29(31.08%) f 6.29(59.31%)g 0.00(0.02%)	6.40
(0.67586) LP (1) N 7 s(2.60%)p37.39(97.26%)d 0.05(0.14%)	(0.13074) LV (2) U 1 s(0.16%)p 2.06(0.32%)d99.99(44.92%) f99.99(54.56%)g 0.30(0.05%)	30.13
(0.67586) LP (1) N 7 s(2.60%)p37.39(97.26%)d 0.05(0.14%)	(0.17176) LV (1) U 2 s(2.59%)p 0.02(0.05%)d12.41(32.17%) f25.15(65.16%)g 0.01(0.02%)	12.51
(0.67586) LP (1) N 7 s(2.60%)p37.39(97.26%)d 0.05(0.14%)	(0.08880) LV (3) U 2 s(24.11%)p 0.02(0.44%)d 1.54(37.05%) f 1.59(38.33%)g 0.00(0.07%)	7.64
(0.66349) LP (2) N 7 s(0.88%)p99.99(98.97%)d 0.16(0.14%)	(0.16017) LV (1) U 1 s(9.44%)p 0.02(0.15%)d 3.29(31.08%) f 6.29(59.31%)g 0.00(0.02%)	25.59
(0.66349) LP (2) N 7 s(0.88%)p99.99(98.97%)d 0.16(0.14%)	(0.17176) LV (1) U 2 s(2.59%)p 0.02(0.05%)d12.41(32.17%) f25.15(65.16%)g 0.01(0.02%)	10.83
(0.67284) LP (1) N 9 s(2.84%)p34.15(97.02%)d 0.05(0.14%)	(0.13074) LV (2) U 1 s(0.16%)p 2.06(0.32%)d99.99(44.92%) f99.99(54.56%)g 0.30(0.05%)	24.24
(0.67284) LP (1) N 9 s(2.84%)p34.15(97.02%)d 0.05(0.14%)	(0.17176) LV (1) U 2 s(2.59%)p 0.02(0.05%)d12.41(32.17%) f25.15(65.16%)g 0.01(0.02%)	19.15
(0.67284) LP (1) N 9 s(2.84%)p34.15(97.02%)d 0.05(0.14%)	(0.06690) LV (4) U 2 s(0.38%)p 5.14(1.97%)d64.04(24.49%) f99.99(73.03%)g 0.34(0.13%)	6.88
(0.66325) LP (2) N 9 s(1.37%)p71.77(98.48%)d 0.11(0.14%)	(0.16017) LV (1) U 1 s(9.44%)p 0.02(0.15%)d 3.29(31.08%) f 6.29(59.31%)g 0.00(0.02%)	27.49
(0.66325) LP (2) N 9 s(1.37%)p71.77(98.48%)d 0.11(0.14%)	(0.17176) LV (1) U 2 s(2.59%)p 0.02(0.05%)d12.41(32.17%) f25.15(65.16%)g 0.01(0.02%)	7.29
(0.66325) LP (2) N 9 s(1.37%)p71.77(98.48%)d 0.11(0.14%)	(0.16502) LV (2) U 2 s(0.06%)p18.07(1.09%)d99.99(7.87%) f99.99(90.96%)g 0.38(0.02%)	9.42
(0.95522) BD (1) U 2- N 7 (18.21%) 0.4268* U 2 s(6.81%)p 0.06(0.41%)d	(0.16017) LV (1) U 1 s(9.44%)p 0.02(0.15%)d 3.29(31.08%) f 6.29(59.31%)g 0.00(0.02%)	6.88

6.61(44.99%) f 7.01(47.75%)g 0.01(0.04%) (81.79%) 0.9044* N 7 s(47.75%)p 1.09(52.15%)d 0.00(0.10%)		
(0.95695) BD (1) U 2- N 9 (18.36%) 0.4285* U 2 s(6.62%)p 0.06(0.41%)d 6.72(44.46%) f 7.33(48.48%)g 0.01(0.04%) (81.64%) 0.9036* N 9 s(47.08%)p 1.12(52.82%)d 0.00(0.10%)	(0.16017) LV (1) U 1 s(9.44%)p 0.02(0.15%)d 3.29(31.08%) f 6.29(59.31%)g 0.00(0.02%)	6.50
(0.96154) BD (1) U 1- N 9 (17.95%) 0.4237* U 1 s(8.38%)p 0.04(0.30%)d 5.82(48.76%) f 5.08(42.53%)g 0.00(0.04%) (82.05%) 0.9058* N 9 s(48.64%)p 1.05(51.27%)d 0.00(0.09%)	(0.08880) LV (3) U 2 s(24.11%)p 0.02(0.44%)d 1.54(37.05%) f 1.59(38.33%)g 0.00(0.07%)	3.40
(0.96184) BD (1) U 1- N 7 (18.30%) 0.4278* U 1 s(7.66%)p 0.04(0.30%)d 6.11(46.75%) f 5.91(45.26%)g 0.00(0.04%) (81.70%) 0.9039* N 7 s(48.70%)p 1.05(51.21%)d 0.00(0.09%)	(0.08880) LV (3) U 2 s(24.11%)p 0.02(0.44%)d 1.54(37.05%) f 1.59(38.33%)g 0.00(0.07%)	2.99

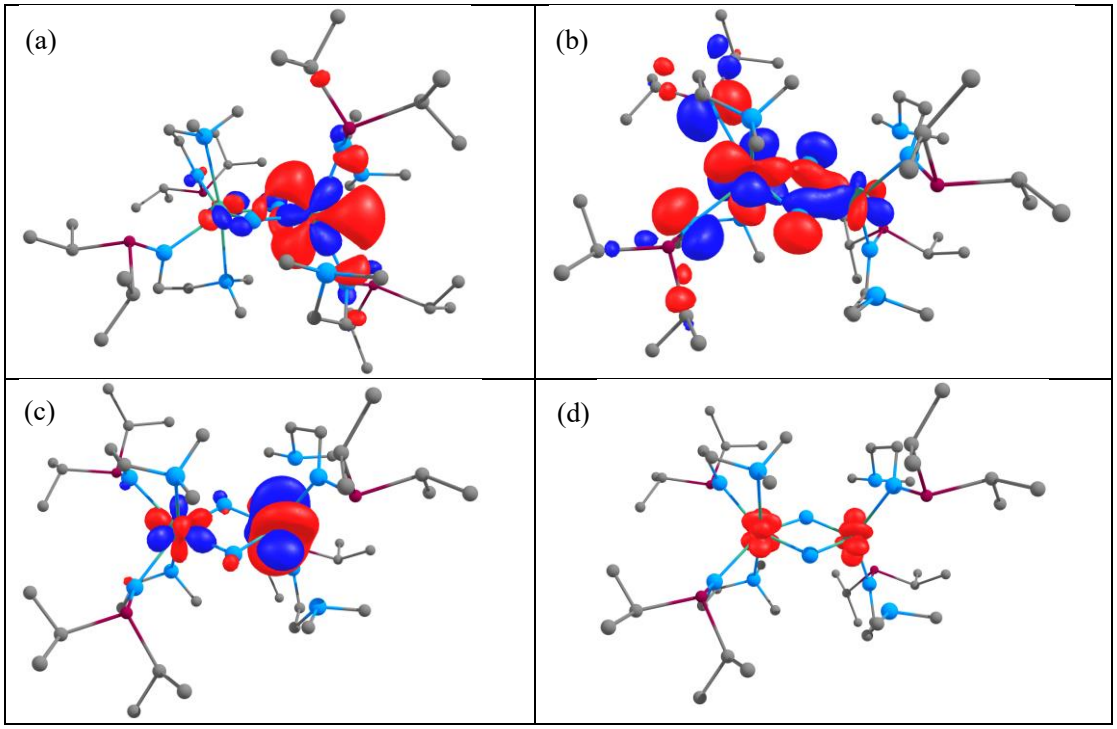


Figure S21. Computed MO's for **4** (s=1). (a) HOMO-1 (b) HOMO (c) LUMO (d) spin density plot (s=1)

Computed 100 states, solvent=THF

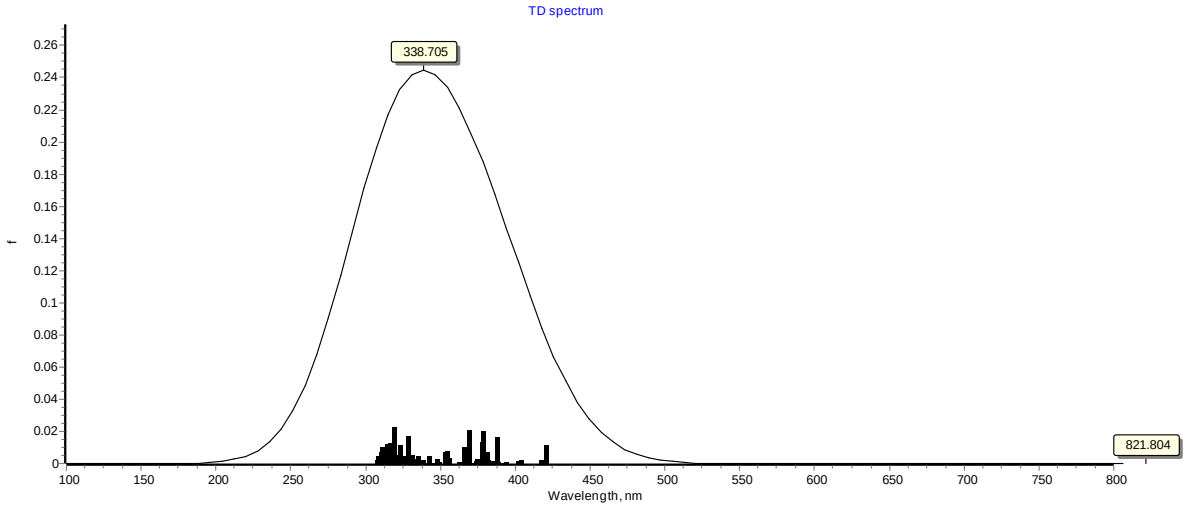


Figure S22. TD spectrum for **3 (s=2)**

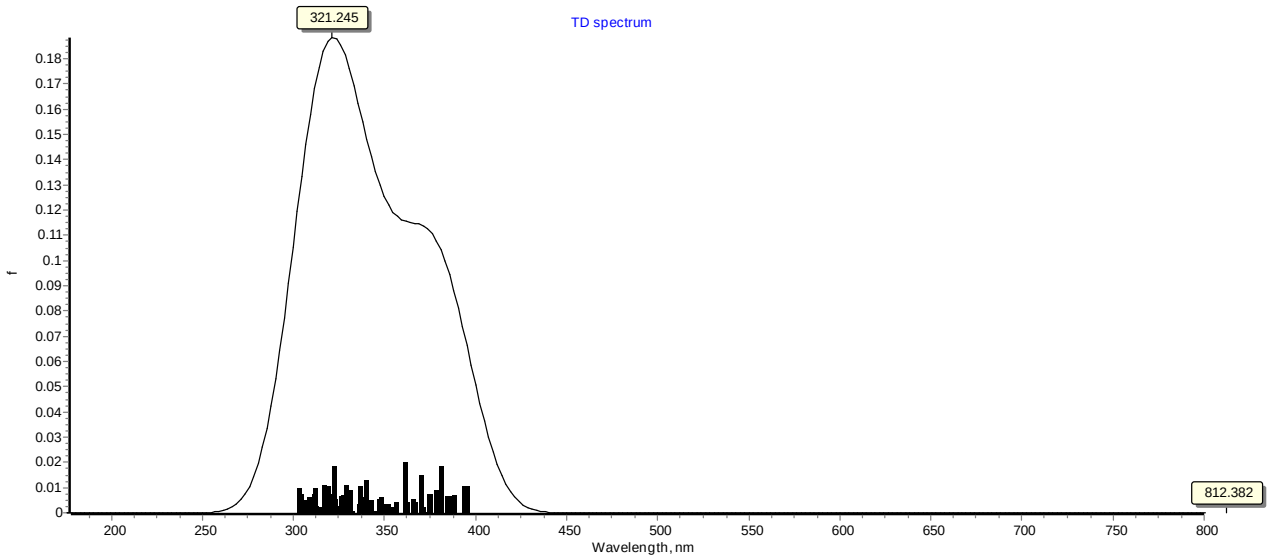


Figure S23. TD spectrum for **3 (s=0, open-shell singlet)**

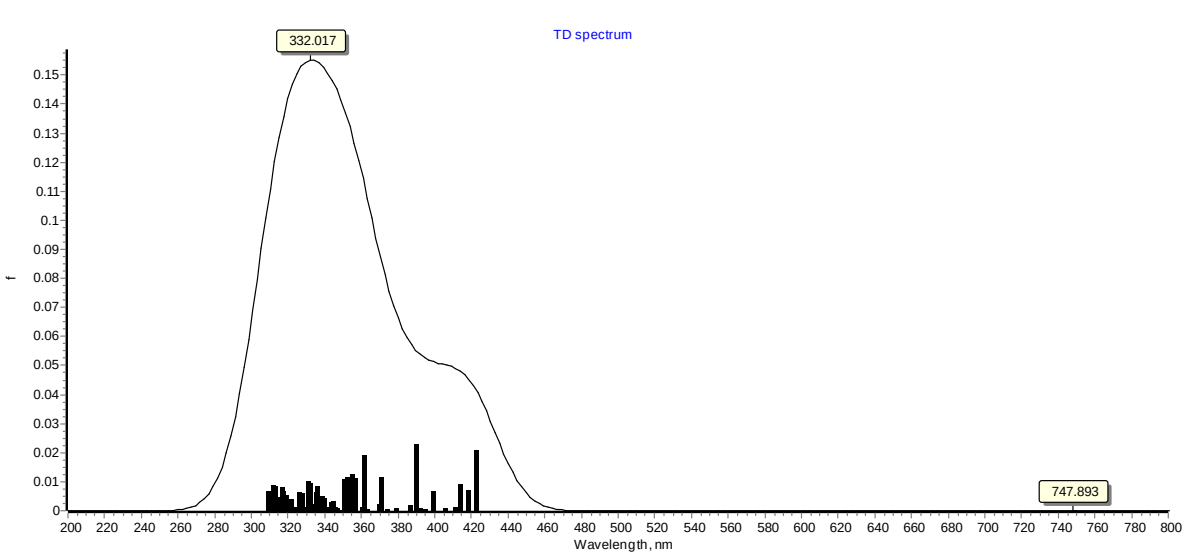


Figure S24. TD spectrum for **3 (s=1)**

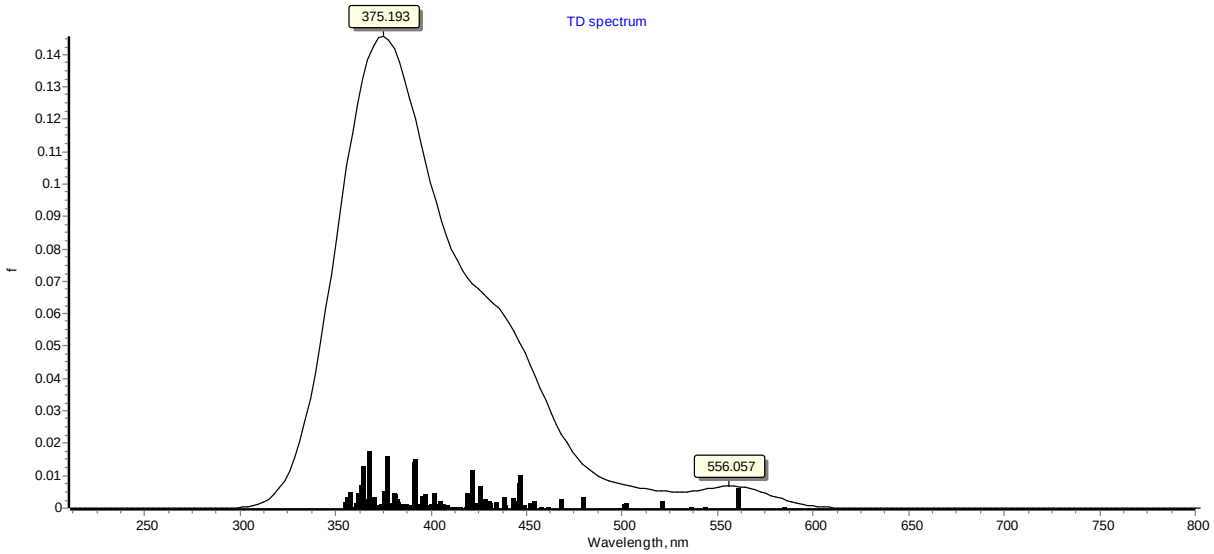


Figure S25. TD spectrum for **4 (s=1)**

Optimized geometries

L_2UCl_2, 1 (s=1)

U	3.014177000	5.330403000	7.150185000
P	4.939630000	7.906904000	6.561850000
N	3.260362000	7.477985000	6.501258000
N	0.621402000	6.672680000	6.918236000
C	0.972186000	8.107981000	6.963406000
H	1.195911000	8.354816000	8.006017000
H	0.112371000	8.720203000	6.645122000
C	-0.331293000	6.384258000	8.002008000
H	-0.634844000	5.336594000	7.954716000
H	-1.230125000	7.014398000	7.912414000
H	0.137959000	6.575339000	8.969793000
C	5.490019000	8.505433000	4.833801000
H	6.546667000	8.751373000	5.011434000
C	2.200318000	8.404719000	6.120951000
H	1.964242000	8.317548000	5.049884000
H	2.480163000	9.452761000	6.290241000
C	5.046200000	9.529196000	7.547041000
H	4.395066000	10.260900000	7.052122000
C	4.560437000	9.339792000	8.981473000
H	3.530697000	8.977543000	9.026572000
H	4.607631000	10.295199000	9.520206000
H	5.184819000	8.621189000	9.523761000
C	5.445229000	7.355758000	3.830035000
H	6.006955000	6.484471000	4.180108000
H	5.881690000	7.670152000	2.873088000

H	4.418958000	7.028787000	3.638904000
C	4.794981000	9.746705000	4.273529000
H	3.745643000	9.547496000	4.034644000
H	5.285480000	10.055897000	3.340946000
H	4.831797000	10.602927000	4.953598000
C	-0.019688000	6.340564000	5.634020000
H	0.649672000	6.561073000	4.801371000
H	-0.952461000	6.911608000	5.503805000
H	-0.254822000	5.273884000	5.609803000
C	6.482856000	10.059299000	7.524890000
H	7.189658000	9.319900000	7.921789000
H	6.560981000	10.955001000	8.153886000
H	6.817342000	10.338746000	6.521374000
P	1.088767000	2.753972000	7.738639000
N	2.768051000	3.182870000	7.799153000
N	5.407072000	3.988221000	7.382192000
C	5.056330000	2.552890000	7.337252000
H	4.832793000	2.305835000	6.294653000
H	5.916142000	1.940784000	7.655776000
C	6.360462000	4.276288000	6.298931000
H	6.664012000	5.323960000	6.346079000
H	7.259233000	3.646165000	6.389298000
H	5.891840000	4.084908000	5.330900000
C	0.538397000	2.155466000	9.466688000
H	-0.518278000	1.909627000	9.289073000
C	3.828088000	2.256181000	8.179593000
H	4.064061000	2.343441000	9.250675000
H	3.548283000	1.208118000	8.010369000
C	0.982160000	1.131685000	6.753449000
H	1.633267000	0.399951000	7.248359000
C	1.467942000	1.321110000	5.319027000
H	2.497708000	1.683287000	5.273953000
H	1.420684000	0.365728000	4.780254000
H	0.843614000	2.039782000	4.776769000
C	0.583314000	3.305134000	10.470459000
H	0.021769000	4.176521000	10.120339000
H	0.146727000	2.990822000	11.427376000
H	1.609632000	3.631913000	10.661673000
C	1.233335000	0.914123000	10.026919000
H	2.282691000	1.113240000	10.265795000
H	0.742819000	0.604939000	10.959496000
H	1.196444000	0.057933000	9.346813000
C	6.047352000	4.320765000	8.666701000
H	5.377475000	4.100540000	9.499010000

H	6.980038000	3.749748000	8.797678000
H	6.282488000	5.387448000	8.690716000
C	-0.454512000	0.601627000	6.775578000
H	-1.161284000	1.341058000	6.378683000
H	-0.532662000	-0.294064000	6.146570000
H	-0.789017000	0.322178000	7.779087000
Cl	2.950046000	4.627551000	4.530210000
Cl	3.077830000	6.033423000	9.770126000

$L_2U(N_3)_2$, 2 (s=1)

U	3.013501000	5.329968000	7.148604000
P	4.819786000	7.832078000	6.457856000
N	3.133796000	7.494340000	6.470076000
N	2.691782000	6.028733000	9.379503000
N	0.563555000	6.604028000	6.846039000
N	2.248108000	6.780517000	10.196537000
C	0.836977000	8.050179000	6.958027000
H	0.998069000	8.264392000	8.019449000
H	-0.038434000	8.634183000	6.627628000
C	-0.495384000	6.253168000	7.802492000
H	-0.696993000	5.181840000	7.753148000
H	-1.424802000	6.802681000	7.582217000
H	-0.180502000	6.505290000	8.818059000
C	5.327251000	8.474160000	4.735996000
H	6.414718000	8.595354000	4.841832000
C	2.078819000	8.451490000	6.178150000
H	1.857571000	8.487358000	5.100706000
H	2.345855000	9.476588000	6.471514000
N	1.821510000	7.495526000	11.002640000
C	5.102658000	9.358658000	7.546654000
H	4.553524000	10.199004000	7.104673000
C	4.569851000	9.121120000	8.957319000
H	3.489428000	8.955923000	8.965413000
H	4.776149000	9.993621000	9.589848000
H	5.046639000	8.254027000	9.429998000
C	5.079572000	7.399645000	3.678626000
H	5.574322000	6.456775000	3.931000000
H	5.466867000	7.728649000	2.706071000
H	4.011378000	7.192593000	3.556718000
C	4.732930000	9.816611000	4.309624000
H	3.650556000	9.751452000	4.160026000
H	5.172945000	10.131104000	3.353959000
H	4.927497000	10.616858000	5.029906000
C	0.115751000	6.254371000	5.490597000

H	0.892554000	6.483717000	4.757563000
H	-0.801005000	6.800466000	5.216180000
H	-0.092905000	5.182083000	5.444816000
C	6.595038000	9.699735000	7.567455000
H	7.190403000	8.859085000	7.944649000
H	6.779813000	10.554101000	8.230469000
H	6.981801000	9.966155000	6.578651000
P	1.208865000	2.828972000	7.846243000
N	2.894849000	3.166239000	7.829510000
N	3.335534000	4.631206000	4.917855000
N	5.464032000	4.056843000	7.450043000
N	3.777868000	3.879005000	4.100444000
C	5.190938000	2.610628000	7.338203000
H	5.028748000	2.396490000	6.276932000
H	6.066899000	2.026857000	7.667554000
C	6.522498000	4.407882000	6.493137000
H	6.724073000	5.479208000	6.542569000
H	7.452069000	3.858449000	6.712964000
H	6.207156000	4.155751000	5.477707000
C	0.704885000	2.186182000	9.568822000
H	-0.382610000	2.063933000	9.464521000
C	3.950135000	2.208868000	8.119479000
H	4.172827000	2.172337000	9.196596000
H	3.682644000	1.183975000	7.825808000
N	4.203250000	3.163576000	3.294103000
C	0.923365000	1.302829000	6.757363000
H	1.472609000	0.461906000	7.198117000
C	1.454453000	1.540688000	5.346086000
H	2.535072000	1.704536000	5.336548000
H	1.246145000	0.668933000	4.713186000
H	0.978136000	2.408767000	4.874720000
C	0.952940000	3.260556000	10.626257000
H	0.455743000	4.202604000	10.375606000
H	0.568418000	2.930228000	11.599465000
H	2.021011000	3.469500000	10.745929000
C	1.301027000	0.844107000	9.993839000
H	2.383514000	0.910162000	10.142087000
H	0.862537000	0.528771000	10.949929000
H	1.106239000	0.044018000	9.273438000
C	5.912169000	4.406761000	8.805307000
H	5.135611000	4.177325000	9.538569000
H	6.829120000	3.860888000	9.079539000
H	6.120543000	5.479104000	8.850882000
C	-0.569230000	0.962576000	6.738408000

H	-1.164718000	1.803810000	6.362719000
H	-0.755428000	0.108789000	6.075039000
H	-0.954713000	0.695566000	7.727552000

$[L_2U(N_3)_2]_2$, 3 (s=2)

U	10.264604000	2.132074000	14.870857000
P	8.185030000	4.177367000	16.118740000
P	12.134567000	0.194193000	13.262397000
N	8.408266000	2.459377000	16.107083000
N	12.097670000	1.891751000	13.570795000
N	11.322399000	4.589641000	13.639963000
N	8.594501000	-0.161973000	15.234610000
N	11.827301000	0.647961000	17.703032000
N	8.981150000	2.276137000	12.945687000
N	11.826903000	3.520453000	17.703396000
N	11.543692000	3.542281000	16.561900000
C	12.261512000	0.019448000	11.374133000
H	13.146381000	0.595381000	11.070338000
N	11.206408000	0.618418000	16.705857000
C	9.258050000	-1.471964000	15.263848000
H	9.685557000	-1.690029000	14.282909000
H	8.545625000	-2.272659000	15.523057000
H	10.064730000	-1.462026000	15.999347000
C	11.234484000	5.836187000	14.408114000
H	10.188357000	6.130086000	14.515139000
H	11.778767000	6.653387000	13.904958000
H	11.656002000	5.687269000	15.403662000
C	8.017400000	0.105805000	16.563669000
H	8.825571000	-0.016099000	17.290011000
H	7.232329000	-0.632868000	16.802075000
C	12.742393000	4.227465000	13.493988000
H	13.173927000	4.215209000	14.499859000
H	13.280156000	4.989802000	12.902592000
C	10.708174000	4.821907000	12.327597000
H	10.749179000	3.922767000	11.712076000
H	11.215288000	5.641107000	11.789670000
H	9.658246000	5.093006000	12.461592000
C	6.388579000	4.501457000	15.598187000
H	5.733404000	4.030020000	16.341074000
C	13.851626000	-0.458077000	13.797166000
H	14.490577000	-0.433487000	12.904401000
N	8.295218000	2.404449000	11.979917000
C	8.232652000	4.679744000	17.962233000
H	8.954630000	3.954238000	18.359964000

C	7.537171000	-0.211063000	14.216692000
H	7.025056000	0.748428000	14.146112000
H	6.796522000	-0.993141000	14.453694000
H	7.976647000	-0.432754000	13.241424000
C	7.457733000	1.517803000	16.673894000
H	6.482377000	1.583212000	16.166933000
H	7.265290000	1.710380000	17.739051000
C	6.119222000	6.008792000	15.578566000
H	6.233405000	6.477635000	16.559981000
H	5.092637000	6.203646000	15.242739000
H	6.793722000	6.522256000	14.882602000
C	8.838338000	6.078596000	18.110146000
H	9.810481000	6.150895000	17.612310000
H	8.983074000	6.326892000	19.169202000
H	8.190072000	6.851680000	17.682309000
C	12.925429000	2.855266000	12.865259000
H	12.673090000	2.890555000	11.794435000
H	13.995208000	2.602642000	12.915456000
C	6.931021000	4.549403000	18.754998000
H	6.172627000	5.265486000	18.421074000
H	7.118931000	4.756448000	19.816991000
H	6.494797000	3.548302000	18.691390000
C	13.709707000	-1.906544000	14.273702000
H	13.116594000	-1.954900000	15.194664000
H	14.694628000	-2.340690000	14.489012000
H	13.220708000	-2.549742000	13.535219000
C	6.099749000	3.896906000	14.226268000
H	6.725057000	4.352408000	13.450382000
H	5.052883000	4.076844000	13.949941000
H	6.269342000	2.817507000	14.202160000
C	11.026828000	0.604749000	10.694300000
H	10.123314000	0.045608000	10.963585000
H	11.134279000	0.552749000	9.603475000
H	10.862534000	1.650461000	10.966005000
N	7.630464000	2.523969000	11.037489000
C	12.466247000	-1.439424000	10.961639000
H	13.408490000	-1.855211000	11.330464000
H	12.485534000	-1.518231000	9.867208000
H	11.649279000	-2.077983000	11.318659000
C	14.488295000	0.401119000	14.885389000
H	14.704349000	1.417400000	14.546951000
H	15.435740000	-0.051300000	15.205227000
H	13.840214000	0.476228000	15.764102000
N	12.448408000	0.623302000	18.700124000

N	12.110183000	3.547676000	18.844848000
U	13.389076000	2.137322000	20.535905000
P	15.469983000	4.182527000	19.291263000
P	11.518254000	0.198724000	22.143855000
N	15.245883000	2.464711000	19.300163000
N	11.556334000	1.896376000	21.835859000
N	12.330709000	4.594141000	21.767023000
N	15.058688000	-0.156734000	20.173244000
N	14.680102000	2.292281000	22.454506000
C	11.389348000	0.024742000	24.031909000
H	10.504530000	0.601229000	24.334747000
C	14.395192000	-1.466766000	20.142991000
H	13.966843000	-1.685232000	21.123476000
H	15.107849000	-2.267313000	19.884034000
H	13.589067000	-1.456504000	19.406851000
C	12.419866000	5.840844000	20.999250000
H	13.466113000	6.135363000	20.895045000
H	11.873874000	6.657662000	21.501179000
H	12.001113000	5.691933000	20.002531000
C	15.636911000	0.111330000	18.844697000
H	14.828900000	-0.009380000	18.117980000
H	16.421527000	-0.627865000	18.606443000
C	10.910515000	4.231978000	21.910991000
H	10.480225000	4.219842000	20.904586000
H	10.371924000	4.994221000	22.501766000
C	12.942833000	4.826244000	23.080408000
H	12.899940000	3.927295000	23.696053000
H	12.435334000	5.645973000	23.617179000
H	13.993288000	5.095986000	22.948188000
C	17.265286000	4.506630000	19.816714000
H	17.922228000	4.036845000	19.074327000
C	9.801446000	-0.452743000	21.607313000
H	9.161473000	-0.427072000	22.499314000
N	15.343732000	2.371965000	23.440764000
C	15.427773000	4.686160000	17.447984000
H	14.707351000	3.960384000	17.047972000
C	16.115171000	-0.206090000	21.192033000
H	16.625858000	0.753984000	21.264758000
H	16.857121000	-0.986763000	20.954442000
H	15.675297000	-0.430690000	22.166499000
C	16.197444000	1.523026000	18.735460000
H	17.171786000	1.588102000	19.244462000
H	16.392176000	1.715258000	17.670659000
C	17.533266000	6.014187000	19.838579000

H	17.419823000	6.484174000	18.857621000
H	18.559277000	6.209547000	20.175872000
H	16.857443000	6.526163000	20.534355000
C	14.821569000	6.084603000	17.298464000
H	13.848179000	6.156248000	17.793978000
H	14.679031000	6.332494000	16.239004000
H	15.468235000	6.858314000	17.727589000
C	10.726842000	2.859795000	22.539598000
H	10.977229000	2.895363000	23.610868000
H	9.657288000	2.606680000	22.487536000
C	16.731786000	4.556515000	16.659027000
H	17.488995000	5.272709000	16.995419000
H	16.546984000	4.763753000	15.596530000
H	17.168058000	3.555488000	16.723701000
C	9.943074000	-1.901693000	21.132190000
H	10.537254000	-1.951228000	20.211979000
H	8.958158000	-2.335444000	20.916065000
H	10.430784000	-2.544539000	21.871832000
C	17.553354000	3.900608000	21.188283000
H	16.925808000	4.352997000	21.964204000
H	18.599515000	4.082705000	21.465980000
H	17.386331000	2.820817000	21.210383000
C	12.624003000	0.610540000	24.711193000
H	13.527371000	0.050543000	24.442994000
H	12.516722000	0.560456000	25.802090000
H	12.788138000	1.655937000	24.437912000
N	15.989840000	2.446051000	24.400662000
C	11.184090000	-1.433693000	24.445498000
H	10.241843000	-1.849458000	24.076643000
H	11.164377000	-1.511577000	25.539987000
H	12.001010000	-2.072800000	24.089339000
C	9.166393000	0.405887000	20.517738000
H	8.950837000	1.422653000	20.855003000
H	8.218756000	-0.046201000	20.197843000
H	9.815058000	0.479552000	19.639347000

$[L_2U(N_3)_2]_2$, 3 (s=1)

U	10.258261000	2.170336000	14.866773000
P	8.195060000	4.201623000	16.094353000
P	12.111422000	0.182349000	13.307487000
N	8.402553000	2.484798000	16.107088000
N	12.110317000	1.881471000	13.597699000
N	11.352928000	4.557053000	13.646269000
N	8.593139000	-0.148112000	15.259866000

N	11.839613000	0.690662000	17.697862000
N	8.972313000	2.261784000	12.929211000
N	11.826074000	3.550361000	17.711703000
N	11.543399000	3.568203000	16.572587000
C	12.250462000	-0.021556000	11.422867000
H	13.156904000	0.520810000	11.120555000
N	11.195387000	0.646865000	16.715212000
C	9.252141000	-1.459595000	15.311591000
H	9.686324000	-1.693166000	14.337239000
H	8.534773000	-2.253913000	15.577094000
H	10.052535000	-1.440276000	16.053515000
C	11.258834000	5.816660000	14.395495000
H	10.212163000	6.112083000	14.490420000
H	11.806173000	6.624182000	13.881162000
H	11.675134000	5.684584000	15.395352000
C	8.011918000	0.136604000	16.583635000
H	8.819237000	0.027172000	17.312653000
H	7.227890000	-0.600635000	16.830058000
C	12.776907000	4.201656000	13.509786000
H	13.203663000	4.197489000	14.517631000
H	13.311968000	4.962845000	12.915593000
C	10.745991000	4.774739000	12.326204000
H	10.792464000	3.868938000	11.721674000
H	11.256262000	5.589421000	11.785361000
H	9.694800000	5.044042000	12.451495000
C	6.406139000	4.540376000	15.560865000
H	5.744988000	4.085187000	16.308557000
C	13.809505000	-0.502915000	13.861564000
H	14.448167000	-0.516164000	12.968290000
N	8.260645000	2.281416000	11.972677000
C	8.249357000	4.729448000	17.928982000
H	8.968214000	4.005237000	18.334160000
C	7.539608000	-0.208297000	14.239033000
H	7.033835000	0.753055000	14.149197000
H	6.792566000	-0.980999000	14.486808000
H	7.981690000	-0.451351000	13.270077000
C	7.447907000	1.547701000	16.674215000
H	6.477697000	1.607075000	16.157071000
H	7.246189000	1.752456000	17.735173000
C	6.152013000	6.049888000	15.521783000
H	6.266843000	6.528939000	16.498159000
H	5.128495000	6.249893000	15.179965000
H	6.833680000	6.548476000	14.822048000
C	8.860230000	6.127369000	18.062277000

H	9.834364000	6.190142000	17.567286000
H	9.002686000	6.385342000	19.119268000
H	8.216504000	6.898868000	17.625068000
C	12.959506000	2.825477000	12.892561000
H	12.720985000	2.854296000	11.818407000
H	14.025339000	2.561524000	12.959403000
C	6.946316000	4.611914000	18.721459000
H	6.191399000	5.328442000	18.380702000
H	7.135144000	4.827413000	19.781516000
H	6.506289000	3.612018000	18.666523000
C	13.628202000	-1.936185000	14.369410000
H	13.036577000	-1.948455000	15.292240000
H	14.601148000	-2.393182000	14.591685000
H	13.119422000	-2.580685000	13.645448000
C	6.114685000	3.919228000	14.196998000
H	6.744839000	4.358528000	13.415775000
H	5.069603000	4.104349000	13.917642000
H	6.274796000	2.838172000	14.188492000
C	11.042870000	0.589057000	10.717601000
H	10.121463000	0.054723000	10.975598000
H	11.168016000	0.524170000	9.629369000
H	10.900045000	1.640828000	10.977537000
N	7.571430000	2.300606000	11.040702000
C	12.412278000	-1.493177000	11.036794000
H	13.334343000	-1.934807000	11.425913000
H	12.443341000	-1.590491000	9.944165000
H	11.568848000	-2.096987000	11.392859000
C	14.471518000	0.363673000	14.928561000
H	14.721019000	1.362912000	14.563496000
H	15.403812000	-0.110277000	15.261566000
H	13.825666000	0.482851000	15.803586000
N	12.483700000	0.678753000	18.682568000
N	12.109461000	3.580713000	18.854432000
U	13.396248000	2.194234000	20.524965000
P	15.453299000	4.218657000	19.304424000
P	11.530039000	0.178144000	22.093267000
N	15.251793000	2.500592000	19.291463000
N	11.565695000	1.883968000	21.822033000
N	12.296013000	4.570942000	21.795991000
N	15.087640000	-0.129350000	20.162201000
N	14.682986000	2.266653000	22.458908000
C	11.410220000	-0.029302000	23.980624000
H	10.531691000	0.547078000	24.301524000
C	14.425638000	-1.439278000	20.121366000

H	14.011918000	-1.673905000	21.104419000
H	15.135151000	-2.235335000	19.839713000
H	13.608588000	-1.417514000	19.397585000
C	12.371871000	5.831819000	21.048647000
H	13.415741000	6.131580000	20.935284000
H	11.831134000	6.637513000	21.573225000
H	11.938734000	5.700117000	20.055785000
C	15.655564000	0.151213000	18.831593000
H	14.843228000	0.029283000	18.110306000
H	16.443399000	-0.581774000	18.583973000
C	10.879435000	4.199905000	21.950141000
H	10.436514000	4.203467000	20.949342000
H	10.344691000	4.947569000	22.562140000
C	12.921761000	4.785553000	23.107037000
H	12.897708000	3.874275000	23.704911000
H	12.412055000	5.590586000	23.663089000
H	13.967939000	5.066987000	22.966510000
C	17.244393000	4.564470000	19.825184000
H	17.903957000	4.112128000	19.074317000
C	9.802280000	-0.453476000	21.564179000
H	9.166020000	-0.428639000	22.458923000
N	15.515130000	2.184934000	23.308886000
C	15.383956000	4.752904000	17.471952000
H	14.661472000	4.029848000	17.070806000
C	16.152104000	-0.188927000	21.170414000
H	16.669775000	0.767688000	21.243677000
H	16.890561000	-0.969747000	20.921685000
H	15.720587000	-0.420858000	22.146932000
C	16.207710000	1.566801000	18.721999000
H	17.183408000	1.638412000	19.227343000
H	16.397016000	1.761739000	17.656530000
C	17.493586000	6.074768000	19.864466000
H	17.374300000	6.553948000	18.888686000
H	18.517365000	6.278327000	20.203509000
H	16.812174000	6.570663000	20.566421000
C	14.770672000	6.150762000	17.348615000
H	13.802753000	6.211349000	17.856111000
H	14.614826000	6.411653000	16.294172000
H	15.418926000	6.921806000	17.779895000
C	10.720964000	2.814063000	22.552038000
H	10.977417000	2.833521000	23.622540000
H	9.655795000	2.542784000	22.501603000
C	16.679365000	4.637395000	16.666963000
H	17.438295000	5.351626000	17.003756000

H	16.481891000	4.857048000	15.609258000
H	17.118140000	3.636519000	16.714733000
C	9.927811000	-1.900302000	21.077504000
H	10.517526000	-1.948575000	20.154364000
H	8.937794000	-2.322907000	20.862111000
H	10.412504000	-2.554181000	21.809276000
C	17.543349000	3.943274000	21.187205000
H	16.907475000	4.372598000	21.969546000
H	18.586095000	4.139048000	21.468061000
H	17.396149000	2.860424000	21.192205000
C	12.652674000	0.534979000	24.664198000
H	13.550403000	-0.027886000	24.383111000
H	12.549743000	0.467245000	25.754753000
H	12.825678000	1.583032000	24.406787000
N	16.317576000	2.108409000	24.141827000
C	11.197076000	-1.493208000	24.370366000
H	10.245841000	-1.892963000	24.006892000
H	11.191411000	-1.591598000	25.463461000
H	12.002611000	-2.133599000	23.991083000
C	9.170197000	0.416735000	20.482251000
H	8.969125000	1.434995000	20.823830000
H	8.215162000	-0.022694000	20.166385000
H	9.813948000	0.485503000	19.599799000

$[L_2U(N_3)_2]_2$, 3 (s=0), open-shell singlet

U	10.270280000	2.098229000	14.870721000
U	13.411011000	2.234087000	20.524627000
N	8.956870000	2.230334000	12.965361000
N	8.260535000	2.360954000	12.007429000
N	7.585611000	2.482628000	11.072539000
N	11.864260000	3.550176000	17.677184000
N	11.571824000	3.537124000	16.540573000
N	12.156312000	3.610538000	18.816763000
N	11.876461000	0.681644000	17.677869000
N	11.247577000	0.618051000	16.684088000
N	12.503974000	0.690546000	18.669106000
N	14.669300000	2.294002000	22.476776000
N	15.474928000	2.134176000	23.341377000
N	16.252110000	1.982421000	24.187410000
P	8.200336000	4.150020000	16.141803000
N	8.428976000	2.431955000	16.129065000
N	8.605115000	-0.191597000	15.256379000
C	9.272723000	-1.499649000	15.279713000
H	9.688287000	-1.718811000	14.293876000

H	8.565714000	-2.301713000	15.549433000
H	10.088139000	-1.486038000	16.005486000
C	8.047389000	0.078092000	16.593391000
H	8.866877000	-0.041973000	17.307129000
H	7.266918000	-0.661182000	16.844881000
C	6.395467000	4.469506000	15.648596000
H	5.751752000	3.994884000	16.399464000
C	8.277347000	4.654090000	17.984228000
H	9.007613000	3.930638000	18.370809000
C	7.532966000	-0.246042000	14.254406000
H	7.017967000	0.712236000	14.188179000
H	6.797762000	-1.028850000	14.505384000
H	7.958279000	-0.469907000	13.273407000
C	7.487513000	1.489602000	16.709740000
H	6.505150000	1.552992000	16.216144000
H	7.309229000	1.683539000	17.777186000
C	6.121878000	5.976222000	15.635081000
H	6.246740000	6.443762000	16.615816000
H	5.090785000	6.169036000	15.312136000
H	6.786498000	6.492684000	14.931885000
C	8.882268000	6.054639000	18.119111000
H	9.845490000	6.128138000	17.604350000
H	9.043995000	6.306436000	19.174861000
H	8.224939000	6.824963000	17.700165000
C	6.990033000	4.522347000	18.799627000
H	6.224758000	5.236923000	18.478527000
H	7.196041000	4.730784000	19.858022000
H	6.554697000	3.520417000	18.744468000
C	6.090652000	3.866483000	14.279377000
H	6.703145000	4.326930000	13.496207000
H	5.039225000	4.041771000	14.017748000
H	6.265535000	2.788033000	14.250394000
P	12.118813000	0.181731000	13.249011000
N	12.081659000	1.881864000	13.537990000
N	11.291188000	4.578260000	13.597867000
C	12.211424000	-0.021125000	11.361719000
H	13.092571000	0.546817000	11.032969000
C	11.208384000	5.829656000	14.357129000
H	10.162060000	6.113592000	14.487528000
H	11.732123000	6.649114000	13.835829000
H	11.655081000	5.694317000	15.343640000
C	12.709795000	4.222113000	13.429097000
H	13.161085000	4.222964000	14.426416000
H	13.232914000	4.980926000	12.820013000

C	10.650006000	4.792368000	12.295902000
H	10.683878000	3.886313000	11.690032000
H	11.141314000	5.608241000	11.738343000
H	9.601308000	5.058988000	12.447474000
C	13.843205000	-0.464901000	13.765326000
H	14.467419000	-0.455016000	12.861934000
C	12.890601000	2.844500000	12.810447000
H	12.620171000	2.868055000	11.743708000
H	13.962743000	2.599335000	12.844828000
C	13.706652000	-1.905427000	14.266903000
H	13.126689000	-1.937773000	15.196849000
H	14.694120000	-2.337299000	14.474951000
H	13.206319000	-2.559803000	13.546029000
C	10.966914000	0.556836000	10.693817000
H	10.066753000	0.004813000	10.987710000
H	11.055504000	0.486210000	9.602345000
H	10.809965000	1.607489000	10.950402000
C	12.403977000	-1.487260000	10.969293000
H	13.350691000	-1.900650000	11.329138000
H	12.404595000	-1.583920000	9.876156000
H	11.590724000	-2.116422000	11.350731000
C	14.497983000	0.410755000	14.829562000
H	14.708459000	1.421424000	14.471249000
H	15.450472000	-0.036343000	15.142253000
H	13.863940000	0.499847000	15.717037000
P	15.514112000	4.219991000	19.333359000
N	15.291130000	2.504635000	19.319179000
N	15.079649000	-0.126397000	20.183423000
C	14.402790000	-1.427903000	20.133583000
H	13.968034000	-1.654246000	21.109535000
H	15.106966000	-2.233943000	19.867205000
H	13.599131000	-1.399089000	19.395160000
C	15.671788000	0.149289000	18.862914000
H	14.870333000	0.040131000	18.127139000
H	16.454077000	-0.592987000	18.625485000
C	17.294985000	4.549399000	19.897355000
H	17.967843000	4.098205000	19.157750000
C	15.496664000	4.744582000	17.496856000
H	14.785624000	4.018697000	17.081068000
C	16.125922000	-0.196322000	21.209540000
H	16.653155000	0.754499000	21.290265000
H	16.860089000	-0.985638000	20.974971000
H	15.675725000	-0.422854000	22.178940000
C	16.244344000	1.557718000	18.766721000

H	17.210574000	1.615119000	19.291472000
H	16.457338000	1.752426000	17.705818000
C	17.549397000	6.058362000	19.948970000
H	17.440718000	6.543372000	18.974729000
H	18.570458000	6.256392000	20.299155000
H	16.862490000	6.552213000	20.646969000
C	14.887867000	6.141216000	17.343687000
H	13.911660000	6.211040000	17.833952000
H	14.748385000	6.384982000	16.282765000
H	15.530729000	6.917845000	17.773205000
C	16.814631000	4.622016000	16.730490000
H	17.564155000	5.337868000	17.084491000
H	16.648014000	4.834468000	15.666080000
H	17.250933000	3.621083000	16.797848000
C	17.563133000	3.918943000	21.261555000
H	16.910329000	4.342775000	22.032862000
H	18.599673000	4.111786000	21.566138000
H	17.415077000	2.836161000	21.255546000
P	11.491928000	0.220585000	22.084573000
N	11.549363000	1.923357000	21.780561000
N	12.317605000	4.601482000	21.767589000
C	11.324402000	0.057079000	23.972579000
H	10.451370000	0.659272000	24.258998000
C	12.437265000	5.862340000	21.024679000
H	13.488473000	6.147988000	20.950098000
H	11.888229000	6.673863000	21.530984000
H	12.038749000	5.737287000	20.016602000
C	10.890748000	4.250932000	21.872880000
H	10.483827000	4.256955000	20.856538000
H	10.345994000	5.008647000	22.462983000
C	12.901252000	4.807216000	23.099776000
H	12.844203000	3.896369000	23.695682000
H	12.383031000	5.618767000	23.637827000
H	13.955095000	5.075016000	22.995339000
C	9.767081000	-0.397549000	21.530084000
H	9.110397000	-0.340462000	22.408374000
C	10.693445000	2.870567000	22.476065000
H	10.913686000	2.893676000	23.554381000
H	9.626939000	2.613387000	22.391469000
C	9.880597000	-1.857680000	21.081723000
H	10.490955000	-1.937828000	20.174333000
H	8.889292000	-2.269968000	20.852851000
H	10.337307000	-2.500782000	21.840542000
C	12.563917000	0.611457000	24.669462000

H	13.454695000	0.022401000	24.421879000
H	12.436584000	0.574075000	25.758879000
H	12.764896000	1.648470000	24.389090000
C	11.070841000	-1.392265000	24.391162000
H	10.118532000	-1.779836000	24.017338000
H	11.040452000	-1.463825000	25.485948000
H	11.869554000	-2.059451000	24.045093000
C	9.174022000	0.455561000	20.413286000
H	8.977390000	1.483652000	20.726622000
H	8.221360000	0.021029000	20.083856000
H	9.839914000	0.497065000	19.545870000

$[L_4U_2(N)_2]$, 4 (s=1)

U	11.787218000	9.627614000	13.829560000
U	11.033893000	11.280010000	16.577090000
P	8.439981000	9.854338000	18.453586000
P	12.903354000	14.136684000	17.241778000
P	11.452348000	10.739545000	10.546763000
P	13.158013000	6.451585000	14.079297000
N	11.630319000	9.453495000	15.859206000
N	9.440459000	8.309363000	13.723294000
N	11.196983000	11.465638000	14.554945000
N	14.231608000	10.725067000	13.607401000
C	11.994924000	10.444966000	20.215153000
H	12.013374000	11.535388000	20.255212000
H	12.700420000	10.059902000	20.972679000
H	10.990925000	10.105736000	20.480905000
N	12.857462000	12.427559000	17.556353000
N	12.331537000	9.968019000	18.874605000
N	10.803704000	9.600605000	11.672703000
N	8.760708000	11.038947000	17.221874000
N	9.297295000	13.532001000	15.988016000
N	13.498016000	8.037909000	13.471013000
C	9.754603000	14.340083000	14.856201000
H	10.658122000	14.885516000	15.140265000
H	8.984280000	15.066953000	14.544679000
H	9.998376000	13.685620000	14.018644000
C	13.706661000	10.334802000	18.517543000
H	13.918874000	9.859445000	17.554774000
H	14.425020000	9.933029000	19.256818000
C	9.473371000	7.690222000	12.385678000
H	8.538747000	7.134459000	12.194506000
H	10.295765000	6.965353000	12.388614000
C	7.134688000	8.662876000	17.690810000

H	7.398970000	8.711531000	16.627592000
C	13.368210000	5.503385000	11.424152000
H	12.274084000	5.428964000	11.392846000
H	13.766701000	4.773558000	10.706830000
H	13.643808000	6.501083000	11.073976000
C	13.897948000	11.840367000	18.388131000
H	13.923334000	12.297497000	19.391787000
H	14.905665000	11.992924000	17.967780000
C	14.923212000	10.689669000	14.900837000
H	14.411057000	11.361170000	15.593330000
H	15.974383000	11.007924000	14.800305000
H	14.896574000	9.682147000	15.318332000
C	13.041361000	15.008307000	18.935035000
H	13.986997000	14.716512000	19.407748000
C	14.303058000	6.224880000	15.607622000
H	14.349761000	7.255231000	15.985494000
C	12.191711000	8.511287000	18.845737000
H	11.156028000	8.241333000	19.069145000
H	12.851965000	8.027609000	19.587010000
H	12.431736000	8.147015000	17.846209000
C	14.633842000	14.475602000	16.472532000
H	14.825007000	13.529186000	15.951173000
C	9.291334000	7.262768000	14.741350000
H	10.116769000	6.551485000	14.660370000
H	8.338810000	6.721793000	14.617112000
H	9.324074000	7.712241000	15.734506000
C	8.119565000	12.753499000	15.585920000
H	8.410117000	12.177159000	14.701833000
H	7.289596000	13.423331000	15.293446000
C	8.164606000	11.934288000	20.364904000
H	9.127329000	11.654492000	20.809211000
H	7.575428000	12.429620000	21.147766000
H	8.364590000	12.673628000	19.585000000
C	13.573885000	3.794459000	13.255265000
H	13.976588000	3.546603000	14.242056000
H	13.990373000	3.071746000	12.541153000
H	12.489408000	3.632426000	13.290841000
C	8.984718000	14.421316000	17.105480000
H	8.719035000	13.845384000	17.993308000
H	8.145617000	15.097264000	16.864941000
H	9.862118000	15.029581000	17.337579000
C	7.425091000	10.713955000	19.824970000
H	6.463972000	11.037702000	19.407734000
C	11.724933000	9.776025000	8.926641000

H	10.767146000	9.336636000	8.619634000
C	13.903479000	5.225352000	12.825091000
H	14.993398000	5.352501000	12.817087000
C	8.330316000	9.262201000	13.840788000
H	8.327145000	9.675502000	14.851542000
H	7.360630000	8.773224000	13.649175000
H	8.459127000	10.083683000	13.134025000
C	5.652653000	9.018984000	17.823901000
H	5.301601000	8.951070000	18.859052000
H	5.045049000	8.316372000	17.236916000
H	5.423835000	10.025223000	17.461626000
C	13.590804000	5.372912000	16.663118000
H	12.587910000	5.753313000	16.881781000
H	14.158580000	5.360193000	17.603234000
H	13.482802000	4.331295000	16.337511000
C	14.848354000	8.387834000	13.059913000
H	15.210232000	7.782686000	12.211912000
H	15.577782000	8.232401000	13.870364000
C	12.209530000	10.715861000	7.821344000
H	11.459091000	11.463358000	7.546229000
H	12.452376000	10.148006000	6.913634000
H	13.118256000	11.252093000	8.123339000
C	14.895573000	9.846421000	12.626114000
H	15.939886000	10.166283000	12.465453000
H	14.360380000	9.966460000	11.677397000
C	10.088536000	11.961525000	9.985027000
H	10.662822000	12.624110000	9.320776000
C	7.397934000	7.231155000	18.168625000
H	8.439449000	6.932966000	18.009351000
H	6.759969000	6.517002000	17.630750000
H	7.184723000	7.113197000	19.237615000
C	15.809982000	14.745621000	17.412902000
H	15.706852000	15.701417000	17.937924000
H	16.744520000	14.800293000	16.837507000
H	15.940574000	13.965704000	18.168452000
C	11.887415000	14.598772000	19.845555000
H	10.923653000	14.923644000	19.436528000
H	11.993701000	15.058497000	20.836710000
H	11.837433000	13.515494000	19.983808000
C	7.646723000	11.802594000	16.677681000
H	7.123755000	12.376072000	17.461417000
H	6.878836000	11.158119000	16.218736000
C	12.720479000	8.643508000	9.161238000
H	13.714532000	9.034680000	9.411020000

H	12.827834000	8.025621000	8.260153000
H	12.403696000	7.994403000	9.981973000
C	7.162627000	9.712090000	20.952700000
H	6.590797000	8.840262000	20.621928000
H	6.594302000	10.184785000	21.764594000
H	8.102455000	9.343844000	21.382421000
C	14.520801000	15.575876000	15.412270000
H	13.727926000	15.362695000	14.687969000
H	15.462444000	15.680847000	14.856927000
H	14.299920000	16.551588000	15.861080000
C	9.705998000	8.723440000	11.294439000
H	9.899371000	8.171460000	10.360725000
H	8.772896000	9.281759000	11.124430000
C	14.221326000	12.104600000	13.106406000
H	13.694788000	12.144159000	12.149499000
H	15.247013000	12.484315000	12.967912000
H	13.694106000	12.744720000	13.816249000
C	13.036927000	16.525032000	18.726329000
H	13.876143000	16.873715000	18.117301000
H	13.095288000	17.046989000	19.690515000
H	12.114070000	16.852954000	18.231757000
C	8.891494000	11.424844000	9.197404000
H	9.180998000	10.763971000	8.374098000
H	8.323246000	12.257060000	8.759407000
H	8.200310000	10.870760000	9.840600000
C	15.730451000	5.723105000	15.382996000
H	15.748239000	4.681886000	15.042284000
H	16.293960000	5.757862000	16.325734000
H	16.282974000	6.319674000	14.651712000
C	9.635824000	12.794900000	11.181709000
H	9.118097000	12.177531000	11.923662000
H	8.944499000	13.588061000	10.867786000
H	10.485102000	13.268585000	11.684732000

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U	11.788155000	9.629782000	13.833455000
U	11.030844000	11.284193000	16.577222000
N	11.643573000	9.459627000	15.860436000
N	11.183908000	11.465512000	14.555030000
P	11.450248000	10.741413000	10.544252000
N	9.447727000	8.310654000	13.727231000
N	10.811524000	9.599271000	11.672444000
C	9.489502000	7.684487000	12.392915000
H	8.558427000	7.123021000	12.201336000

H	10.315295000	6.963670000	12.402994000
C	9.298507000	7.268924000	14.750468000
H	10.127733000	6.561187000	14.677508000
H	8.349179000	6.722865000	14.624385000
H	9.323905000	7.724378000	15.741142000
C	11.722934000	9.777609000	8.924307000
H	10.766078000	9.334022000	8.620475000
C	8.332377000	9.258958000	13.834172000
H	8.320021000	9.675155000	14.843626000
H	7.366569000	8.764584000	13.637191000
H	8.462425000	10.078961000	13.125967000
C	12.200648000	10.718096000	7.816533000
H	11.446431000	11.462155000	7.542392000
H	12.443411000	10.150109000	6.908872000
H	13.107957000	11.258502000	8.115341000
C	10.078022000	11.955225000	9.984459000
H	10.646652000	12.618974000	9.316488000
C	12.723648000	8.649362000	9.157584000
H	13.716944000	9.044797000	9.403641000
H	12.830579000	8.030312000	8.257243000
H	12.411863000	8.000658000	9.980536000
C	9.720216000	8.713014000	11.296501000
H	9.919770000	8.156309000	10.366869000
H	8.784304000	9.264558000	11.120143000
C	8.880508000	11.411077000	9.202659000
H	9.170106000	10.750547000	8.379094000
H	8.306021000	12.239599000	8.765765000
H	8.194915000	10.854193000	9.849462000
C	9.625668000	12.789326000	11.180798000
H	9.112760000	12.171410000	11.925632000
H	8.930159000	13.579051000	10.867401000
H	10.474571000	13.267503000	11.680280000
P	13.162666000	6.451636000	14.082859000
N	14.230701000	10.726844000	13.607938000
N	13.497464000	8.037602000	13.471131000
C	13.358907000	5.502862000	11.426943000
H	12.264411000	5.431552000	11.401810000
H	13.751408000	4.771382000	10.707987000
H	13.635296000	6.499503000	11.074361000
C	14.926891000	10.690091000	14.898992000
H	14.417560000	11.361090000	15.594002000
H	15.977771000	11.008018000	14.794801000
H	14.901282000	9.682264000	15.315751000
C	14.316690000	6.226080000	15.604880000

H	14.364809000	7.256494000	15.982420000
C	13.573144000	3.794166000	13.257389000
H	13.979476000	3.546886000	14.242848000
H	13.986778000	3.070839000	12.542224000
H	12.488770000	3.632378000	13.297148000
C	13.901384000	5.224767000	12.825094000
H	14.991324000	5.351198000	12.811178000
C	13.611111000	5.373746000	16.664567000
H	12.608940000	5.752992000	16.888604000
H	14.183882000	5.361960000	17.601683000
H	13.502494000	4.331905000	16.339871000
C	14.846022000	8.389596000	13.056125000
H	15.206044000	7.785684000	12.206390000
H	15.578207000	8.234352000	13.864104000
C	14.890766000	9.848650000	12.623369000
H	15.934307000	10.168958000	12.458682000
H	14.351674000	9.969182000	11.676933000
C	14.218974000	12.106853000	13.107953000
H	13.689774000	12.147155000	12.152522000
H	15.244282000	12.486477000	12.966649000
H	13.694089000	12.746874000	13.819672000
C	15.743026000	5.725020000	15.372085000
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H	16.312375000	5.761092000	16.311261000
H	16.290587000	6.321014000	14.636609000
P	12.906535000	14.136456000	17.243271000
C	11.990291000	10.444349000	20.214663000
H	12.010056000	11.534745000	20.255147000
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H	10.985807000	10.106224000	20.480074000
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C	13.896614000	11.837553000	18.388411000
H	13.922131000	12.294560000	19.392118000
H	14.904957000	11.988215000	17.968859000
C	13.044623000	15.006310000	18.937432000
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C	12.184910000	8.511044000	18.844274000
H	11.148661000	8.242259000	19.066673000
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C	14.638309000	14.473407000	16.475965000
H	14.828223000	13.527406000	15.953420000
C	15.814133000	14.739762000	17.417743000
H	15.712672000	15.695210000	17.943705000
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C	11.888875000	14.598428000	19.846411000
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C	14.528303000	15.575445000	15.417226000
H	13.735971000	15.364676000	14.691612000
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H	14.308508000	16.550857000	15.867215000
C	13.043909000	16.523236000	18.730262000
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P	8.433801000	9.854963000	18.450868000
N	8.756920000	11.039781000	17.220067000
N	9.298518000	13.533943000	15.989398000
C	9.756601000	14.342934000	14.858386000
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H	8.987404000	15.071820000	14.548928000
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C	7.124887000	8.667746000	17.687639000
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C	8.119468000	12.757725000	15.586024000
H	8.409482000	12.182230000	14.701234000
H	7.290844000	13.429544000	15.294404000
C	8.164788000	11.934001000	20.364206000
H	9.126738000	11.651153000	20.808237000
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H	8.366758000	12.673356000	19.584836000
C	8.987240000	14.422524000	17.107915000
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H	8.149447000	15.100201000	16.867869000
H	9.865715000	15.028925000	17.340853000
C	7.421676000	10.716256000	19.823381000
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C	5.643966000	9.028602000	17.820569000
H	5.292689000	8.962348000	18.855758000
H	5.034159000	8.327647000	17.233888000
H	5.418434000	10.035380000	17.457754000

C	7.383491000	7.235207000	18.165524000
H	8.424385000	6.934125000	18.007583000
H	6.744169000	6.522927000	17.626791000
H	7.168656000	7.117756000	19.234243000
C	7.644563000	11.806091000	16.676227000
H	7.122189000	12.379305000	17.460571000
H	6.875801000	11.163655000	16.215918000
C	7.156571000	9.714226000	20.950320000
H	6.581704000	8.844586000	20.619056000
H	6.590210000	10.188021000	21.762945000
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[$L_4U_2(N)_2$], 4 (s=0), open-shell singlet

U	11.770403000	9.641510000	13.869447000
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P	12.867705000	14.303897000	17.083407000
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P	12.947499000	6.413499000	14.085267000
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H	12.622276000	10.369956000	20.907650000
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C	9.518812000	14.174691000	14.925494000
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H	14.432805000	10.212365000	19.249911000
C	9.514258000	7.818000000	12.250088000
H	8.582682000	7.290951000	11.979789000
H	10.324511000	7.080193000	12.257960000
C	7.200496000	8.458264000	17.791088000

H	7.442566000	8.597394000	16.729369000
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C	13.836184000	12.077420000	18.337019000
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H	14.839229000	12.265804000	17.920964000
C	14.932439000	10.615132000	14.952463000
H	14.449937000	11.329817000	15.621832000
H	15.998346000	10.880671000	14.852369000
H	14.857651000	9.621127000	15.395725000
C	13.124120000	15.267498000	18.714191000
H	14.102078000	15.000742000	19.132871000
C	14.000611000	6.153486000	15.670343000
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C	8.109440000	11.660024000	20.589726000
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C	13.308835000	3.748379000	13.277996000
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H	12.218474000	3.628593000	13.260189000
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C	8.292074000	9.304360000	13.724188000
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C	13.110103000	16.767039000	18.405654000
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H	9.243222000	13.789662000	10.891305000
H	10.728026000	13.383846000	11.770203000

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