Assembling Diuranium Complexes in Different States of Charge with a Bridging Redox-Active Ligand

Dieuwertje K. Modder, [§a] Mikhail S. Batov, [§a] Thayalan Rajeshkumar,[b] Rosario Scopelliti,[a] Ivica Zivkovic,[c] Andrzej Sienkiewicz,[c] Laurent Maron*[b] and Marinella Mazzanti[a]*

[a] Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland.

[b] LPCNO, Université de Toulouse, INSA Toulouse, Toulouse, 31077, France.
[c] Laboratory for Quantum Magnetism, Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland.

E-mail: marinella.mazzanti@epfl.ch
§ D.M and M.B contributed equally to the manuscript
* To whom correspondence should be addressed.

Supporting Information

Contents

Experimental data

General considerations.

All manipulations were carried out under inert nitrogen/argon atmosphere using an MBraun glovebox equipped with a purifier unit and Schlenk line techniques. The water and oxygen levels were always kept at less than 1 ppm. Anhydrous solvents were purchased from Sigma Aldrich and vacuum distilled under potassium/benzophenone (THF, toluene, Et_2O) or sodium sand/benzophenone (hexane). Depleted uranium turnings were purchased from IBILABS, Florida (USA). Bipyrimidine was purchased from Sigma Aldrich and used as received after drying under vacuum for 3 days.

$[U\{N(SiMe_3)_2\}_3]$[1], KC_8[2] and $[K(2.2.2\text{-cryptand})]_2[\{((Me_3Si)_2N)_3U\}_2(\mu\text{-}O)]$[3] were synthesized according to their respective literature procedures. Elemental analyses were performed under nitrogen with a Thermo Scientific Flash 2000 Organic Elemental Analyzer at EPFL. The elemental analyses were reproduced several times on different batches and under different conditions, always giving low values of carbon for complexes **2** and **4** probably due to combustion issues and/or the formation of silicon carbides. However, the C:H:N ratio's match the expected ones.

^1H NMR experiments were carried out using NMR tubes adapted with J. Young valves. ^1H NMR spectra were recorded on a Bruker 400 MHz spectrometer and the chemical shifts are reported in ppm with residual proteo-solvent signals used as an internal reference.

Cyclic voltammetry experiments were carried out at room temperature in an argon-filled glovebox described above. Data were collected using a Biologic SP-300 potentiostat connected to a personal computer. All samples were 2 mM in complex with 0.06 M $[NBu_4][BPh_4]$ supporting electrolyte in THF solution. The experiments were carried out with a platinum disk (d = 5 mm) working electrode, a platinum wire counter electrode, and an Ag/AgCl reference electrode. The experiments were repeated on independently synthesized samples to assess the reproducibility of the measurement. Potential calibration was performed at the end of each data collection cycle using the decamethylferrocene/decamethylferrocenium $[(C_5Me_5)_2Fe]^{+/0}$ couple as an internal standard. The values were subsequently adjusted to reflect the values versus the $[(C_5H_5)_2Fe]^{+/0}$ couple assuming that $[(C_5Me_5)_2Fe]^{+/0}$ appears at –0.59 V with respect to $[(C_5H_5)_2Fe]^{+/0}$.

Electron paramagnetic resonance (EPR) measurements were recorded with a Bruker Elexsys E500 spectrometer operating in the X-band frequency region with an Oxford ESR900 cryostat for 4-300 K operation. The complexes were ground in an agate mortar. 5 mmol were loaded in 1 mm diameter quartz capillaries and then inserted into J-Young valve EPR tubes. The measurements were reproduced from at least two different synthetic batches.

Magnetic measurements were performed using a QuantumDesign MPMS3 system operating at temperatures 2–300 K. Quartz tubes were charged with solid samples of each complex, which were ground using an agate mortar and pestle. Solid eicosane was added,

and the tubes were fit with a Teflon sealable adapter, evacuated under vacuum, and flame-sealed under static vacuum. Following flame sealing, the solid eicosane was melted in a water bath at 40 °C, and the mixture was immediately cooled with an ice bath. Diamagnetic corrections were applied to the data using tabulated Pascal constants.[4] The measurements were reproduced from at least two different synthetic batches. The sample were vacuum dried before the measurements to remove solvents.

AC measurements were performed using the same experimental setup in the range of frequencies up to 1 kHz under the applied field of 0.2 T. Relaxation parameters for **2** and **4** were extracted by least squares fitting of the Argand (Cole-Cole) plots using the generalised Debye model[5]. For compound **3** no maximum was observed on the Argand plot and therefore no further analysis was attempted. The energy barrier values for **2** and **4** were obtained from the linear fit of the Arrhenius plot (ln(τ) against 1/T)[5]. Attempts to include Raman or direct processes in the fit did not yield a better fit.

Caution: *Depleted uranium (primary isotope ^{238}U) is a weak α-emitter (4.197 MeV) with a half-life of 4.47×10^9 years. Manipulations and reactions should be carried out in monitored fume hoods or in an inert atmosphere glovebox in a radiation laboratory equipped with α- and β-counting equipment.*

Syntheses.

[{((Me$_3$Si)$_2$N)$_3$U}$_2$(μ-bpym)] (1). A solution of 2,2'-bipyrimidine (109.9 mg, 0.695 mmol, 1 eq) in THF (1 mL) was added to a purple solution of [U{N(SiMe$_3$)$_2$}$_3$] (1000 mg, 1.39 mmol, 2 eq) in THF (1 mL). An immediate color change to dark green/brown, as well as the formation of a crystalline precipitate was observed. The reaction mixture was stirred for 2h at room temperature. Then the green precipitate was collected by filtration, washed with hexane (2x3 mL) and Et$_2$O (2x3 mL) until washings were colorless, and dried under vacuum for 30 minutes, to yield a light green solid (686.2 mg, 62%). Complex **1** is insoluble in hexane and Et$_2$O and only slightly soluble in toluene and THF. Anal. Calcd. for $C_{44}H_{114}N_{10}Si_{12}U_2$: C, 33.10; H, 7.20; N, 8.77. Found: C, 33.10; H, 7.39; N, 8.52. ^{1}H-NMR (400 MHz, THF-d_8, 298K): δ 33.98 (s), -7.70 (br s) and -23.48 (br s). X-ray quality crystals were obtained by carrying out the reaction on a small scale (10 mg of [U{N(SiMe$_3$)$_2$}$_3$]) and crystallize out upon addition of 2,2'-bipyrimidine without stirring.

[K(2.2.2-cryptand)][{((Me$_3$Si)$_2$N)$_3$U}$_2$(μ-bpym)] (2). A suspension of **1** (100 mg, 0.063 mmol, 1 eq) and 2.2.2-cryptand (23.6 mg, 0.063 mol, 1 eq) in THF (1 mL) was added to KC_8 (8.5 mg, 0.063 mmol, 1 eq). After stirring at room temperature for 2h, the color changed from light green to black-green. The mixture was filtered, affording a dark brown solution. All volatiles were removed under vacuum and diffusion of hexane into a concentrated Et$_2$O solution −40 °C for 5 days resulted in the formation of X-ray suitable black crystals (92.7 mg,

73%) which were subsequently washed with additional hexane (1x2 ml) and dried under vacuum for 30 minutes. Anal. Calcd. for $C_{62}H_{150}KN_{12}O_6Si_{12}U_2$: C, 37.01; H, 7.51; N, 8.35. Found: C, 34.76; H, 6.94; N, 7.85. ^{1}H-NMR (400 MHz, THF-d_8, 298K): δ 13.05 (s), 3.57 (s, 2.2.2-cryptand), 3.53 (s, 2.2.2-cryptand), 2.54 (s, 2.2.2-cryptand), -8.80 (br s).

[K(2.2.2-cryptand)]$_2$[{((Me$_3$Si)$_2$N)$_3$U}$_2$(μ-bpym)] (3). From [K(2.2.2-cryptand)]$_2$ [{((Me$_3$Si)$_2$N)$_3$U}$_2$(μ-O)] NMR scale. A (−80 °C) solution of bipyrimidine (0.8 mg, 5.1 μmol, 1.2 eq) in THF-d_8 (0.5 mL) was added to [K(2.2.2-cryptand)]$_2$[{((Me$_3$Si)$_2$N)$_3$U}$_2$(μ-O)] (9.9 mg, 4.3 μmol, 1.0 eq), resulting in a dark brown solution. The variable temperature ^{1}H-NMR spectra showed complete conversion of the starting materials at −80 °C and the formation of the side product [K(2.2.2-cryptand)][U(O){N(SiMe$_3$)$_2$}$_3$] and at 0 °C the formation of complex **3** was observed (complex **3** is silent at lower temperatures). **From complex 1.** A suspension of **1** (100 mg, 0.062 mmol, 1 eq) and 2.2.2-cryptand (47 mg, 0.125 mol, 2 eq) in THF (1 mL) was added to KC_8 (16.9 mg, 0.125 mmol, 2 eq). After stirring for 2h at room temperature, the black reaction mixture was filtered and all volatiles were removed under vacuum. The residue was dissolved in minimal Et_2O and the resulting solution was cooled to −40 °C, affording dark brown crystals suitable for X-ray diffraction. The crystals were collected and dried under vacuum for 30 minutes. Anal. Calcd. for $C_{80}H_{186}K_2N_{14}O_{12}Si_{12}U_2$: C, 39.58; H, 7.72; N, 8.08. Found: C, 39.12; H, 7.42; N, 8.26. ^{1}H-NMR (400 MHz, THF-d_8, 298K): δ 12.79 (s), 3.48 (s, 2.2.2-cryptand), 3.45 (s, 2.2.2-cryptand), 2.46 (s, 2.2.2-cryptand), -7.37 (br s).

[{((Me$_3$Si)$_2$N)$_3$U}$_2$(μ-bpym)][BPh$_4$] (4). An off-white suspension of $AgBPh_4$ (53.4 mg, 0.125 mmol, 1 eq) in THF (1 mL) was added to a stirring suspension of **1** (200 mg, 0.125 mmol, 1 eq) in THF (1 mL) and stirred at room temperature for 3h, resulting in a dark brown mixture. The mixture was filtered and slow diffusion of hexane into the THF reaction mixture at −40 °C over 3 days afforded X-ray quality brown crystals. The resulting brown crystals were washed with toluene (3x2 ml) and hexane (3x2 ml) and dried under vacuum for 30 minutes to yield complex **4** (148.6 mg, 62%) as a brown powder. ^{1}H-NMR (400 MHz, THF-d_8, 298K): δ 7.42, 6.97 and 6.77 (all s, 20H, B*Ph$_4$*), -21.46 and -24.84 (two s, broad, 54H, NSi*Me$_3$*). Anal. Calcd. for $C_{68}H_{134}BN_{10}Si_{12}U_2$: C, 42.63; H, 7.05; N, 7.31. Found: C, 41.71; H, 6.37; N, 6.96. For **5**, ^{1}H-NMR (400 MHz, THF-d_8, 298K): δ 7.48 (s, B*Ph$_4$*), 6.90 (s, B*Ph$_4$*), 6.56 (s, B*Ph$_4$*), -13.49 (s) and -19.51 (s).

NMR Spectra

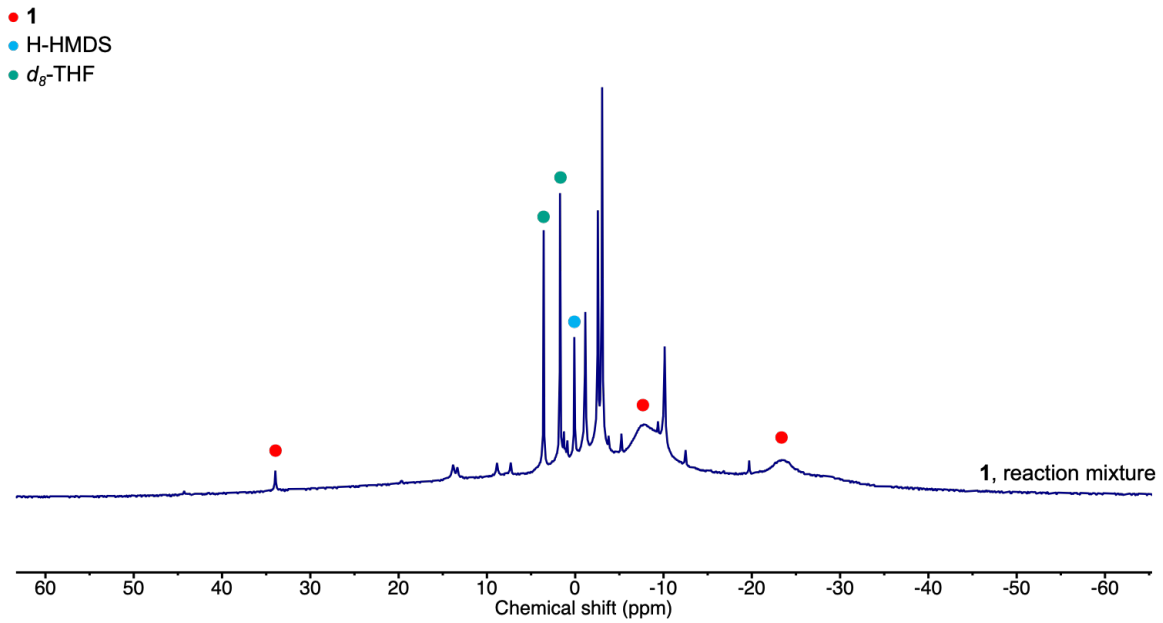

Figure S1 Room temperature ^{1}H-NMR spectrum of reaction mixture in THF-d_8 of the reaction mixture of $[U\{N(SiMe_3)_2\}_3]$ and 0.5 equivalents of 2,2'-bipyrimidine, forming complex **1**.

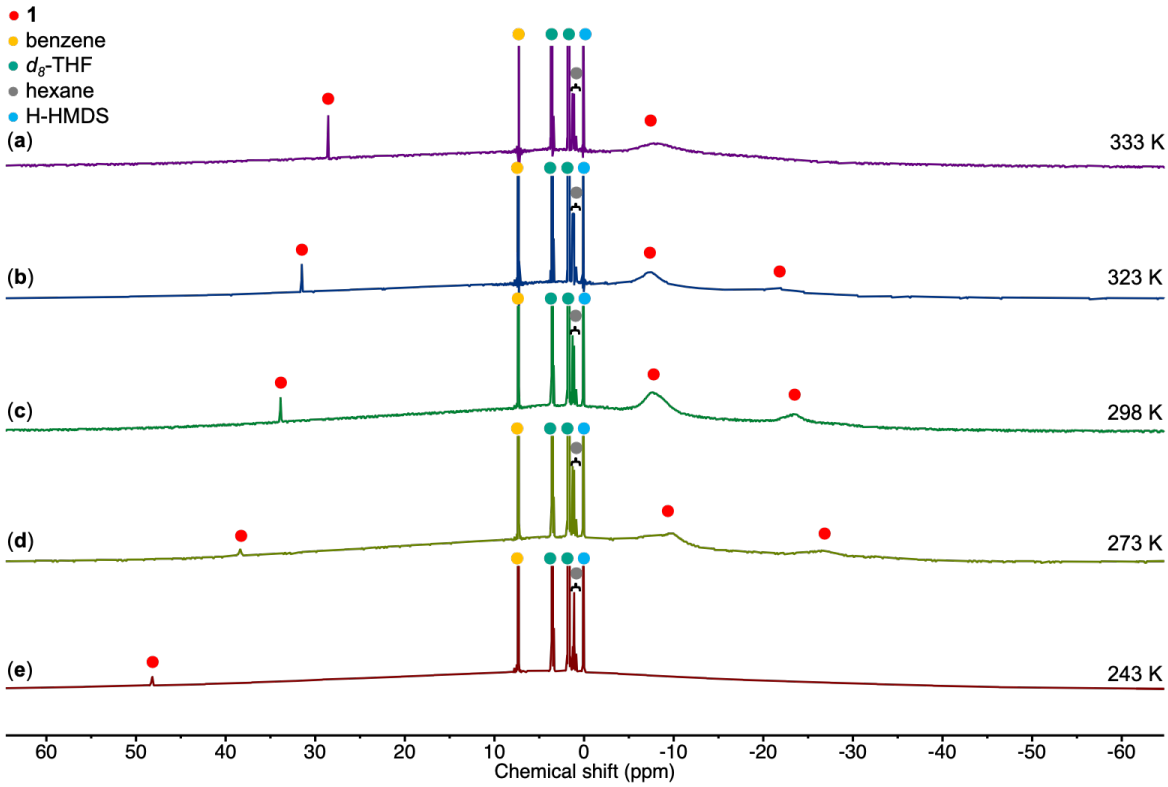

Figure S2 Variable temperature ^{1}H-NMR spectra of crystals of **1** in THF-d_8 (a-e).

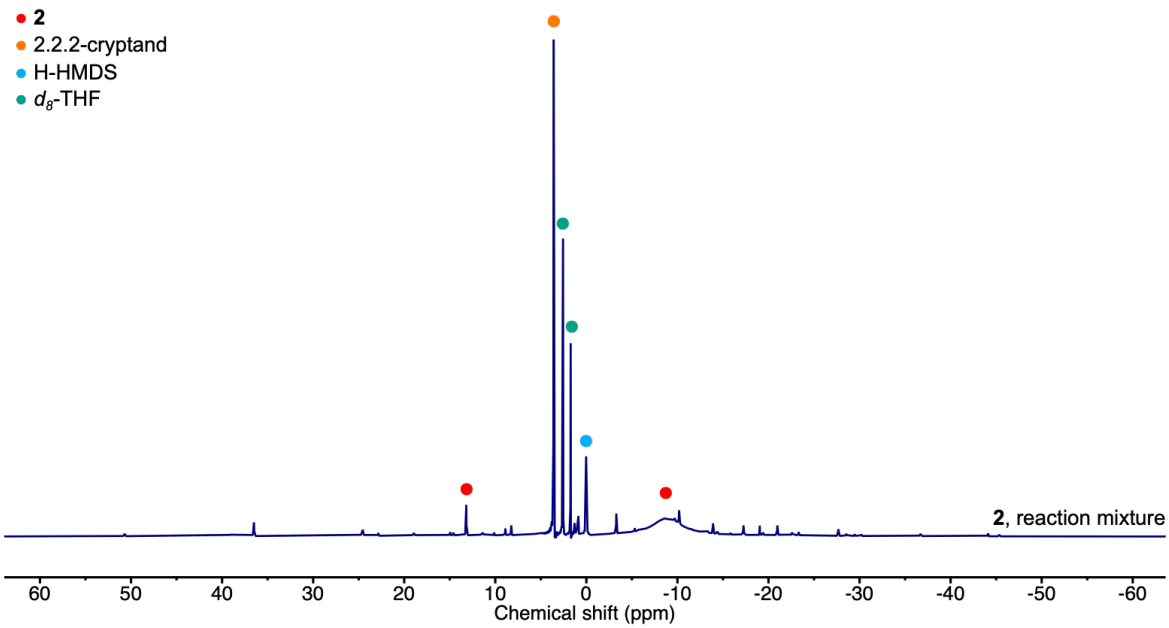

Figure S3 Room temperature ^{1}H-NMR spectrum of the reaction mixture in THF-d_8 of complex **1** with 1 equivalent of KC_8 and 1 equivalent of 2.2.2.-cryptand, forming complex **2**.

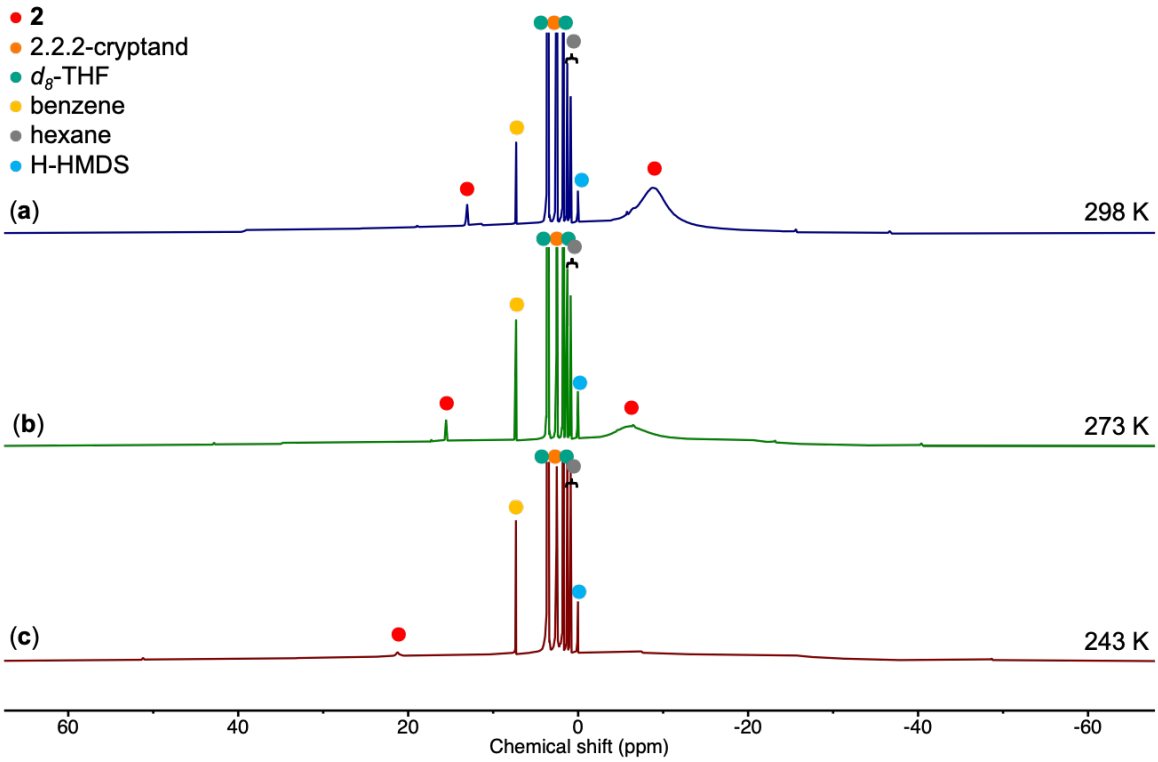

Figure S4 Variable temperature ^{1}H-NMR spectra of crystals of **2** in THF-d_8 (a-c).

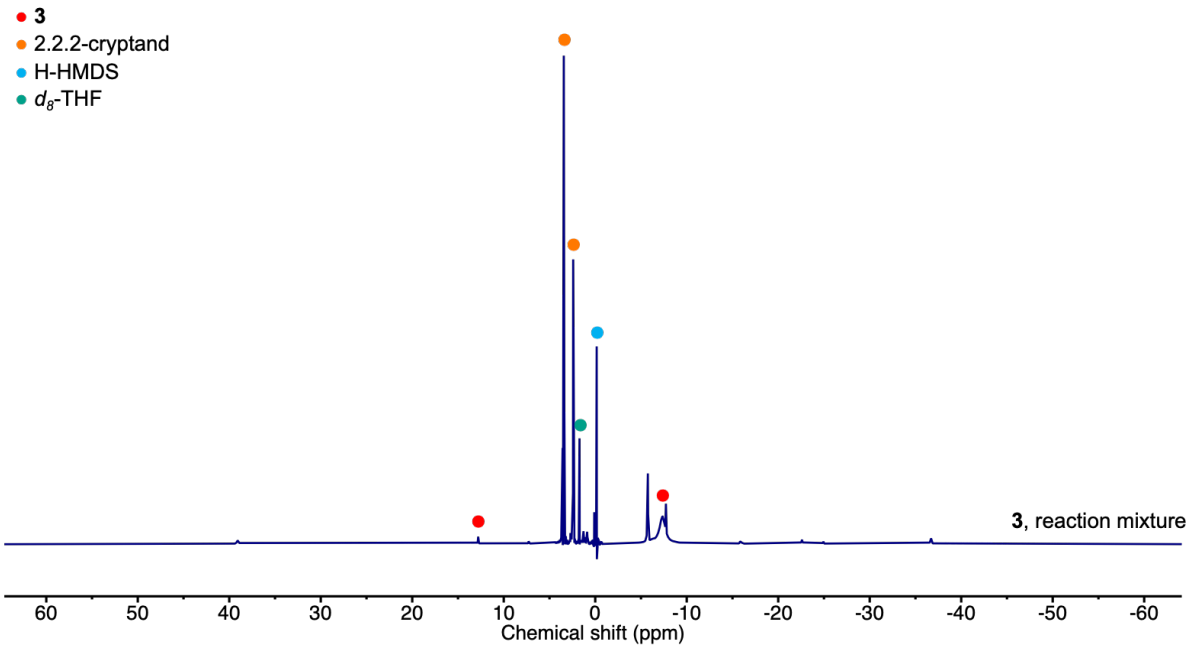

Figure S5 Room temperature ^{1}H-NMR spectrum of the reaction mixture in THF-d_8 of complex **1** with 2 equivalents of KC_8 and 2 equivalents of 2.2.2-cryptand, forming complex **3**.

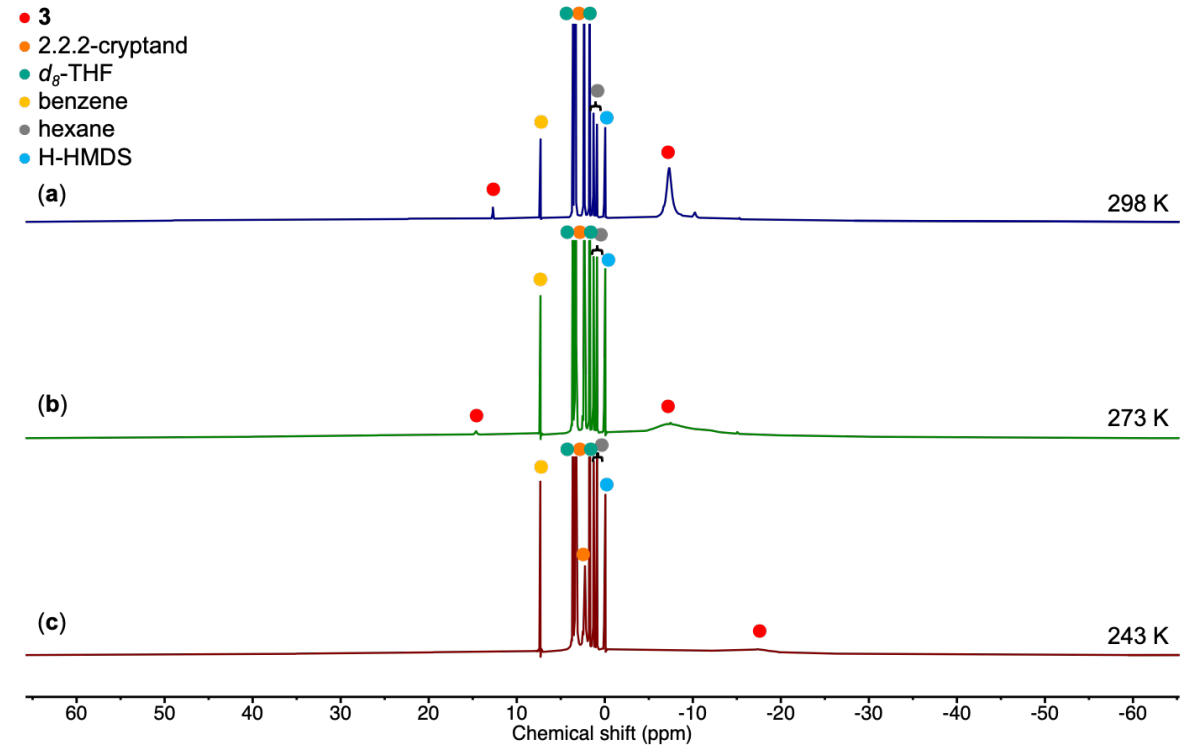

Figure S6 Variable temperature ^{1}H-NMR spectra of crystals of **3** in THF-d_8 (a-c).

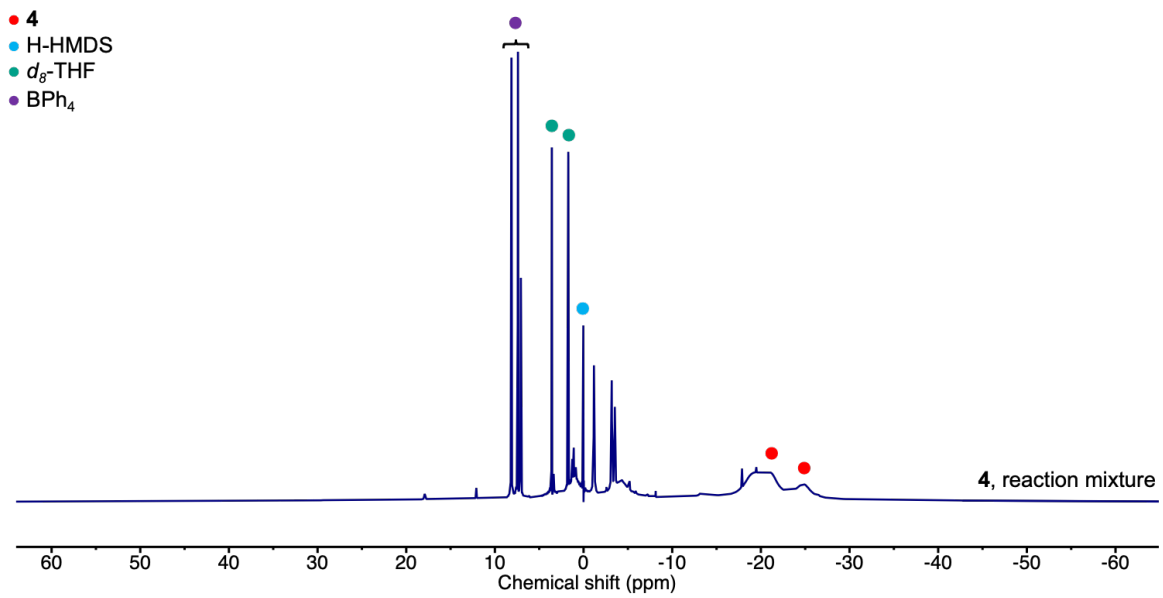

Figure S7 Room temperature ^{1}H-NMR spectrum of the reaction mixture in THF-d_8 of complex **1** and $AgBPh_4$, forming complex **4**.

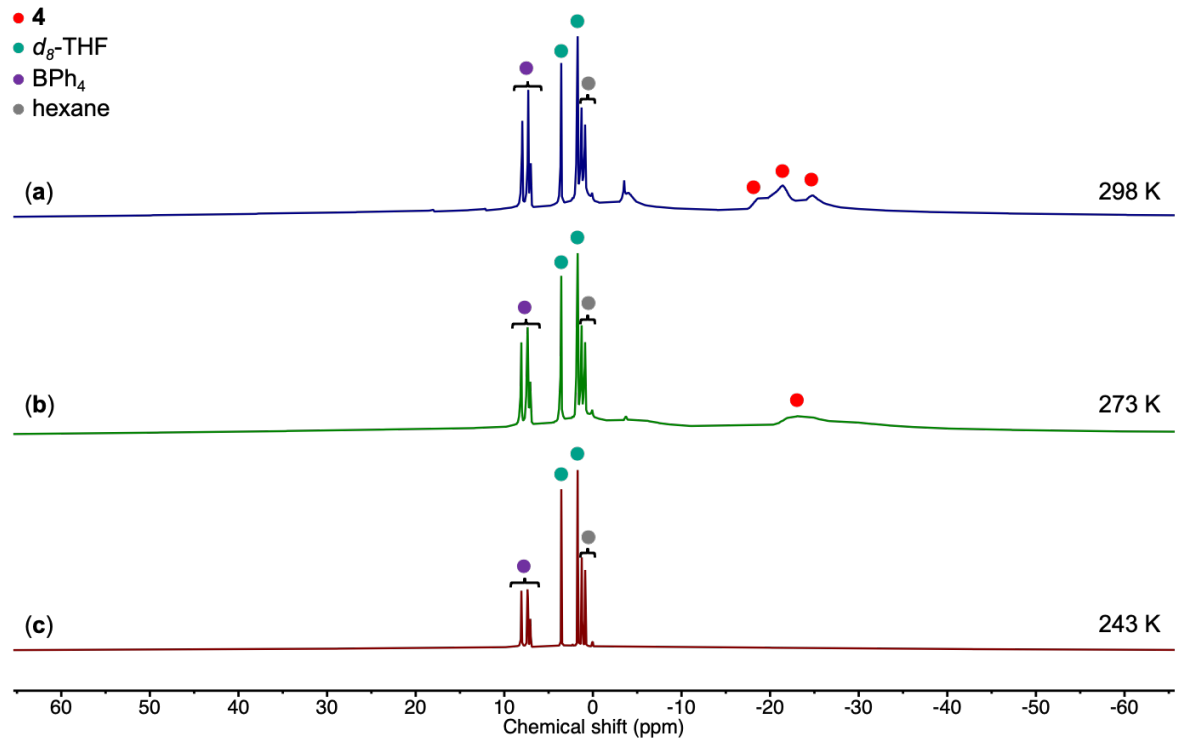

Figure S8 Variable temperature ^{1}H-NMR spectra of crystals of **4** in THF-d_8 (a-c).

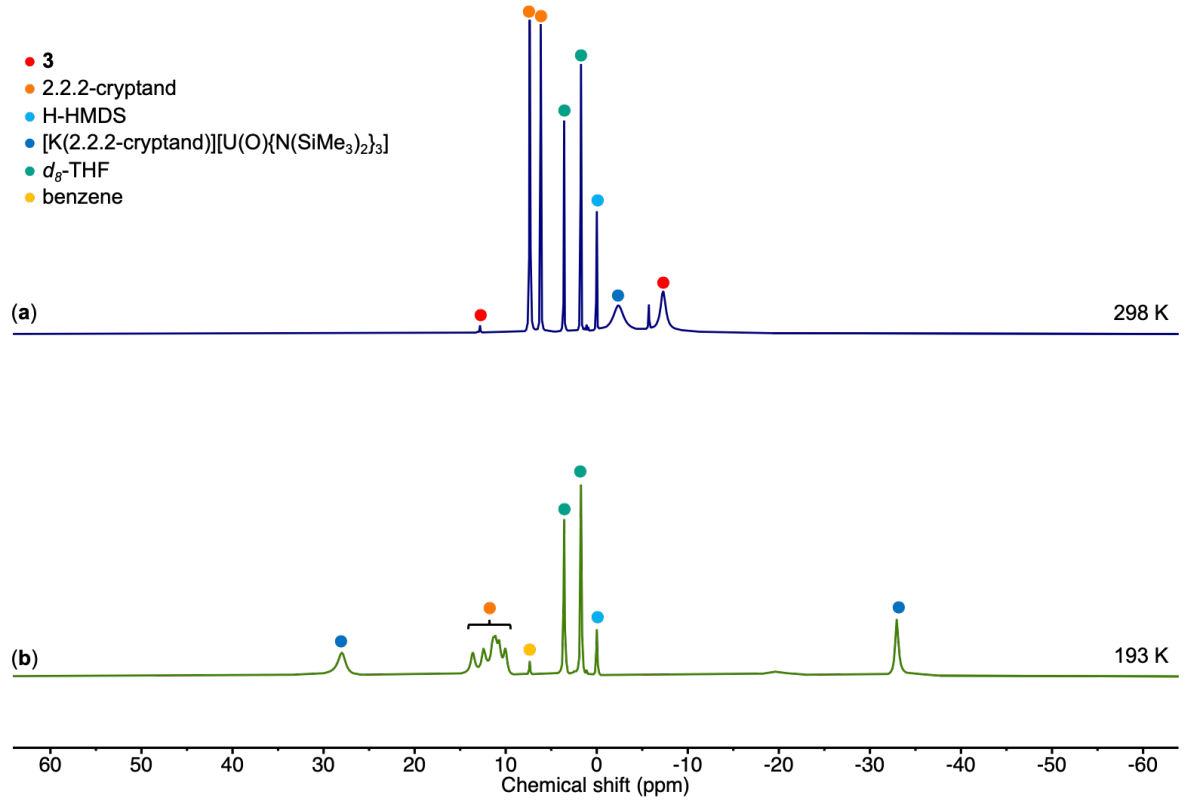

Figure S9 ^{1}H-NMR spectra of reaction mixture of [K(2.2.2-cryptand)]$_2$[{((Me$_3$Si)$_2$N)$_3$U}$_2$(μ-O)] with 1 equivalent of 2,2'-bipyrimidine in THF-d_8 yielding **3**, along with the side-product [K(2.2.2-cryptand][U(O){N(SiMe$_3$)$_2$}$_3$] (a-b).

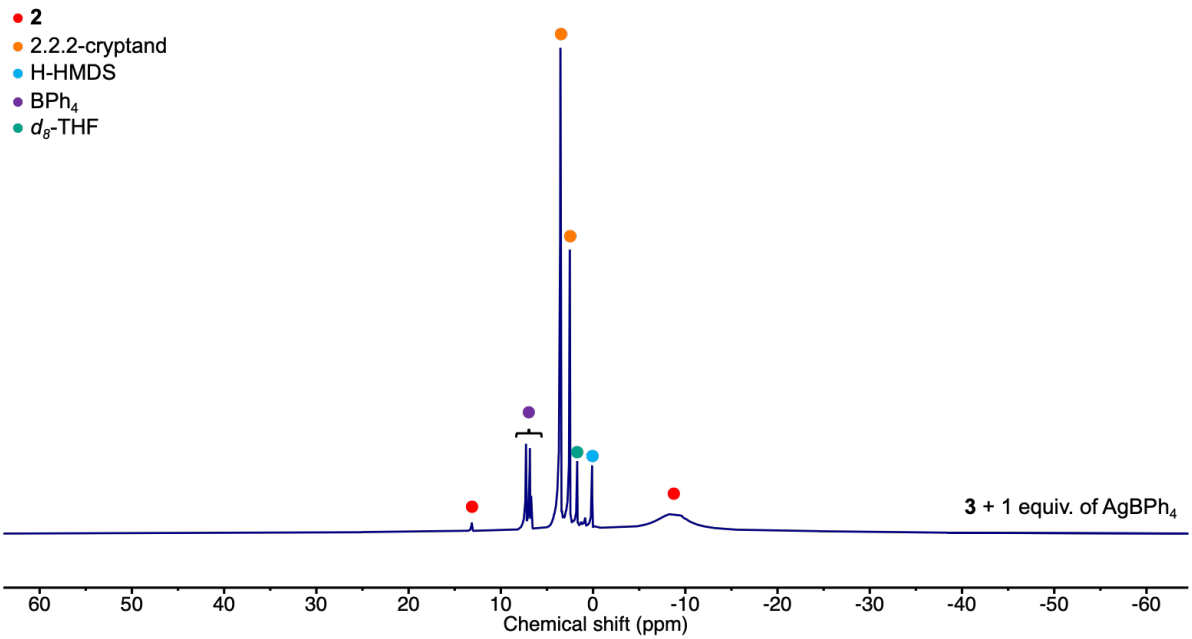

Figure S10 ^{1}H-NMR spectra of reaction mixture of **3** with 1 equivalent of AgBPh$_4$ in THF-d_8 yielding **2**.

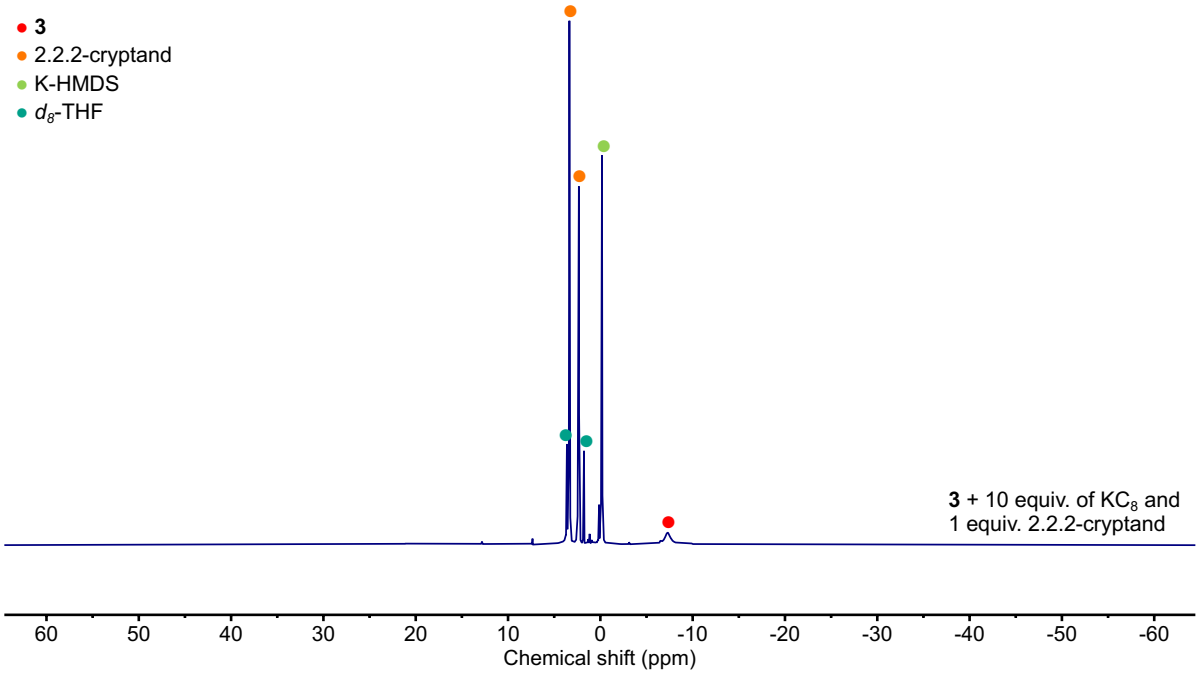

Figure S11 ^{1}H-NMR spectrum of reaction mixture of **3** with 10 equivalents of KC_8 and 1 equiv. 2.2.2-cryptand in THF-d_8 resulting in the partial decomposition of **3** to K-HMDS.

X-ray Structure and Refinement Details

Suitable crystals were selected and mounted on various Rigaku diffractometers (XtaLAB Synergy R, DW system, HyPix-Arc 150 detector or SuperNova, Dual, Cu at home/near, AtlasS type detectors). The crystals were kept at a steady T = 140.00(10) K during data collection. Data were measured using □ scans with Cu K□ radiation. The diffraction patterns were indexed and the total number of runs and images were based on the strategy calculation from the program CrysAlisPro 1.171.41.118a (Rigaku OD, 2021).[6] The unit cells were refined using CrysAlisPro 1.171.41.118a (Rigaku OD, 2021). Data reduction, scaling and absorption corrections were performed using CrysAlisPro 1.171.41.118a (Rigaku OD, 2021).

The structures were solved with the **ShelXT**[7] (Sheldrick, 2015) solution program using dual methods and by using **Olex2** 1.5[8] as the graphical interface. The models were refined with **ShelXL**[9] 2018/3 using full matrix least squares minimisation on F^2. All non-hydrogen atoms were refined anisotropically. Some hydrogen atom positions were calculated geometrically and refined using the riding model, but most hydrogen atoms were refined freely.

Several structures displayed problems dealing with disorder (disordered ligands or solvent) or twinning. In particular, the crystal structure of compound **1** was treated for twinning (2 BASF parameters (0.144(1); 0.377(2)) were refined during the last cycles of least-squares) and the solvent was removed from the model (using Olex2). For compound **2** several restraints (cards: SADI, DFIX, RIGU, ISOR) were needed to adjust the atomic parameters of the K(crypt)$^+$ and the solvent (0.5 hexane) was squeezed in the last stages of the refinement (using Olex2). The crystal structure of compound **4** showed one disordered ligand and restraints were used for its refinement (cards: SADI, SIMU, RIGU), solvent too was highly disordered and it was removed from the model (using Olex2). In the case of compound **5**, the solvent was removed from the model (using Olex2).

Table S1 X-ray data for complexes **1-4**.

Complex	**1**	**2**	**3**	**4**
Formula	$C_{44}H_{114}N_{10}Si_{12}U_2$	$C_{62}H_{150}KN_{12}O_6Si_{12}U_2$	$C_{96}H_{226}K_2N_{14}O_{16}Si_{12}U_2$	$C_{71}H_{141}BN_{10}Si_{12}U_2$
$D_{calc.}$/ g cm^{-3}	1.333	1.308	1.332	1.203
m/mm^{-1}	13.339	10.903	8.674	9.910
Formula Weight	1596.59	2012.17	2724.23	1958.88
Colour	clear dark green	black	clear dark brown	black
Shape	prism	irregular	irregular	prism-shaped
Size/mm^3	0.26×0.11×0.10	0.31×0.07×0.05	0.27×0.14×0.11	0.41×0.15×0.11
T/K	140.00(10)	140.00(10)	139.9(9)	140.00(10)
Crystal System	monoclinic	monoclinic	triclinic	triclinic
Space Group	*I*2/*a*	*I*2/*a*	$P\bar{1}$	*P*-1
a/Å	24.4164(5)	29.9688(16)	13.78160(13)	15.1222(2)
b/Å	11.4199(2)	11.6805(5)	16.73893(18)	15.2178(2)
c/Å	29.7959(6)	32.306(3)	17.00630(17)	23.8147(4)
a/°	90	90	63.8536(11)	98.8987(12)
b/°	106.683(2)	115.332(9)	84.3138(8)	91.1267(12)
g/°	90	90	74.6504(9)	92.6498(13)
V/Å^3	7958.4(3)	10221.3(14)	3395.39(7)	5406.63(14)
Z	4	4	1	2
Z'	0.5	0.5	0.5	1
Wavelength/Å	1.54184	1.54184	1.54184	1.54184
Radiation type	Cu K$_\alpha$	Cu K$_\alpha$	Cu K$_\alpha$	Cu K$_\alpha$
Q_{min}/°	4.143	3.027	2.895	2.926
Q_{max}/°	72.828	73.679	76.054	76.884
Measured Refl's.	9407	37255	40729	66393
Ind't Refl's	9407	10025	14025	22270
Refl's with I > 2s(I)	8306	6715	13728	17947
R_{int}	.	0.0827	0.0276	0.0426
Parameters	327	447	662	990
Restraints	0	446	0	385
Largest Peak	1.408	2.844	1.510	1.842
Deepest Hole	-1.839	-2.447	-1.402	-1.573
GooF	1.018	1.019	1.021	1.021
wR_2 (all data)	0.0879	0.2502	0.0536	0.1041
wR_2	0.0861	0.2026	0.0532	0.0959
R_1 (all data)	0.0359	0.1091	0.0227	0.0551
R_1	0.0320	0.0771	0.0221	0.0411
CCDC	2181473	2181474	2181478	2181475

Table S1 continued.

Complex	**5**
Formula	$C_{34}H_{48}KN_{10}O_6$
$D_{calc.}$/ g cm^{-3}	1.175
m/mm^{-1}	1.551
Formula Weight	731.92
Colour	black
Shape	irregular-shaped
Size/mm^3	0.16×0.13×0.12
T/K	140.01(10)
Crystal System	monoclinic
Space Group	$C2/c$
a/Å	15.3683(13)
b/Å	20.5260(10)
c/Å	14.6910(10)
a/°	90
b/°	116.777(9)
g/°	90
V/Å^3	4137.3(6)
Z	4
Z'	0.5
Wavelength/Å	1.54184
Radiation type	Cu K$_\alpha$
Q_{min}/°	3.875
Q_{max}/°	72.755
Measured Refl's.	16648
Ind't Refl's	4046
Refl's with I > 2s(I)	3014
R_{int}	0.0364
Parameters	241
Restraints	2
Largest Peak	0.331
Deepest Hole	-0.212
GooF	1.027
wR_2 (all data)	0.1259
wR_2	0.1144
R_1 (all data)	0.0591
R_1	0.0420
CCDC	2181476

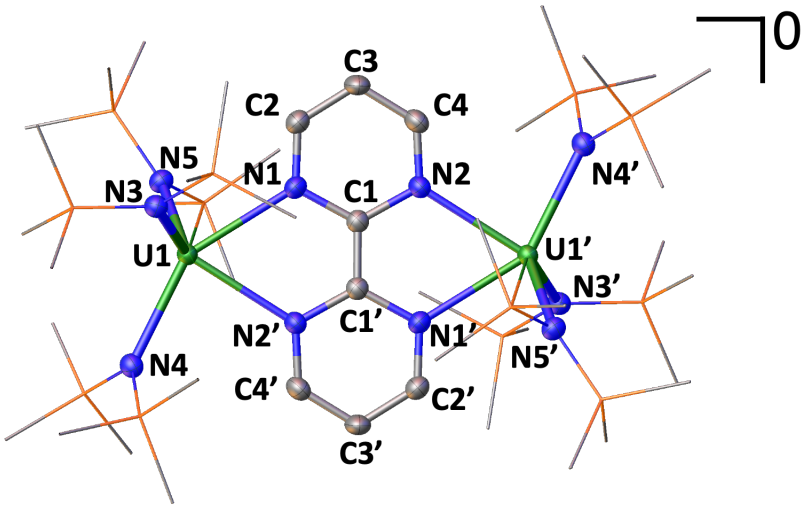

Figure S12. Molecular structure of **1**, with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms and [K(2.2.2-cryptand)] counter cation have been omitted for clarity. Selected bond lengths (Å): U1–$(N_{amide})_{avg}$ 2.285(9), U1–N1 2.518(4), U1–N2 2.499(4), N1–C1 1.411(6), N2–C1 1.410(6), N1–C2 1.323(6), N2–C4 1.3334(6), C2–C3 1.401(7), C3–C4 1.392(7), C1–C1' 1.344(9).

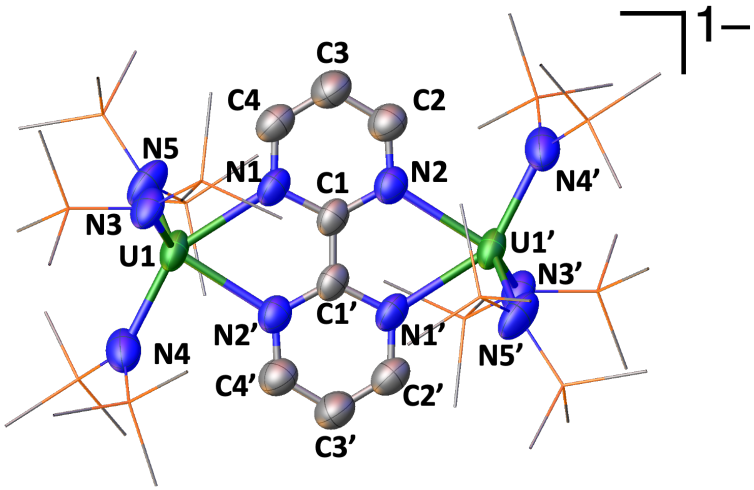

Figure S13. Molecular structure of **2**, with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms and [K(2.2.2-cryptand)] counter cation have been omitted for clarity. Selected bond lengths (Å): U1–$(N_{amide})_{avg}$ 2.36(1), U1–N1 2.494(1), U1–N2 2.516(9), N1–C1 1.406(13), N2–C1 1.401(15), N1–C4 1.349(17), N2–C2 1.321(17), C2–C3 1.39(2), C3–C4 1.38(2), C1–C1' 1.37(2).

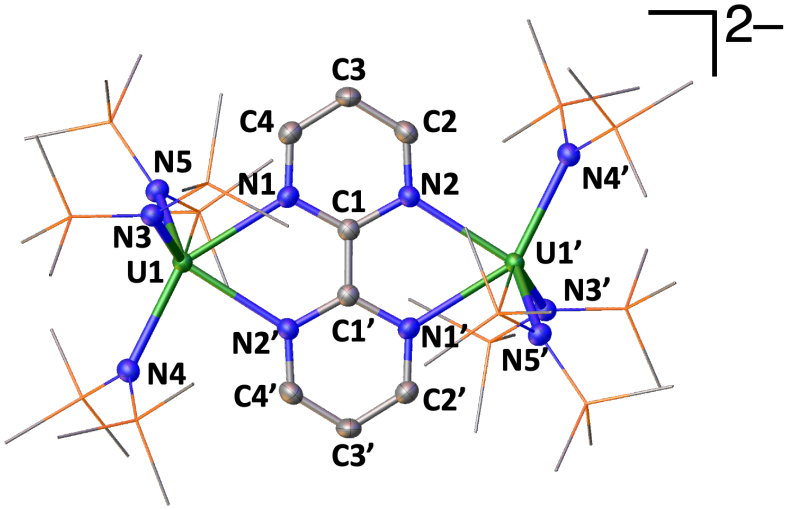

Figure S14. Molecular structure of **3**, with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms and [K(2.2.2-cryptand)] counter cations have been omitted for clarity. Selected bond lengths (Å): U1–$(N_{amide})_{avg}$ 2.44(4), U1–N1 2.567(2), U1–N2 2.562(2), N1–C1 1.432(2), N2–C1 1.420(3), N1–C4 1.319(3), N2–C2 1.312(2), C2–C3 1.404(3), C3–C4 1.396(3), C1–C1' 1.349(5).

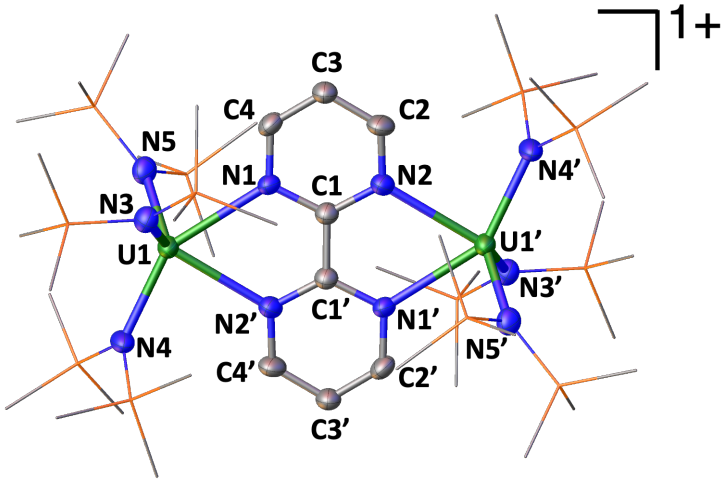

Figure S15. Molecular structure of **4**, with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms and [BPh_4] counter cations have been omitted for clarity. Selected bond lengths (Å): U1–$(N_{amide})_{avg}$ 2.258(6), U1–N1 2.553(5), U1–N2 2.604(5), N1–C1 1.386(7), N2–C1 1.363(7), N1–C4 1.338(7), N2–C2 1.337(7), C2–C3 1.386(8), C3–C4 1.381(8), C1–C1' 1.405(10), U2–$(N_{amide})_{avg}$ 2.25(1), U2–N6 2.557(4), U1–N7 2.585(5), N6–C23 1.395(7), N7–C23 1.367(7), N6–C26 1.334(7), N7–C24 1.333(7), C24–C25 1.402(8), C25–C26 1.389(8), C23–C23' 1.409(10).

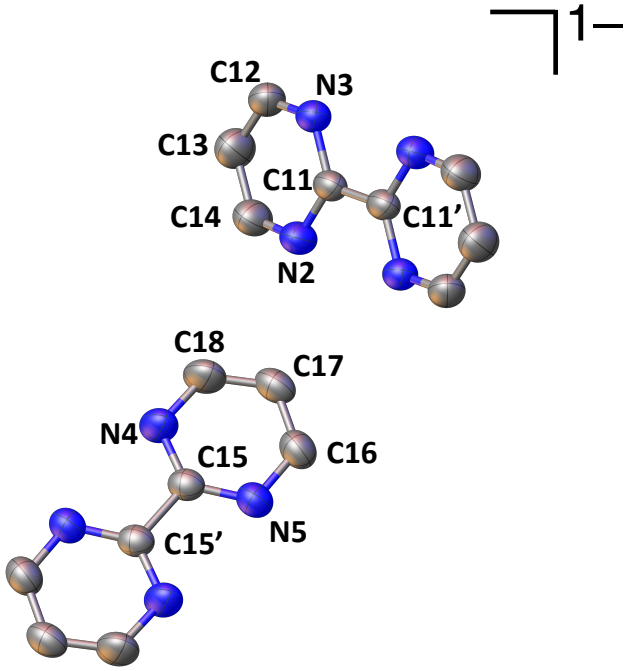

Figure S16. Molecular structure of **5** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms and [K(2.2.2-cryptand)] counter cation have been omitted for clarity. Selected bond lengths (Å): C11–C11' 1.423(4), N3–C11 1.380(3), N3–C12 1.316(3), C12–C13 1.388(3), C13–C14 1.390(3), N2–C14 1.308(3), N2–C11 1.371(2), C15–C15'1.506(3), N5–C15 1.339(3), N5–C16 1.334(3), C16–C17 1.365(3), C17–C18 1.359(3), N4–C18 1.339(3), N4–C15 1.320(3).

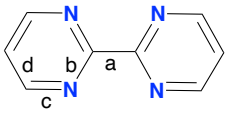

Table S2 Comparison of averaged bond lengths of complexes **1-5**, with **5** split into bpym^{0} and bpym$^{\bullet-}$.

Bond	**1**	**2**	**3**	**4**	**5**-bpym^{0}	**5**-bpym$^{\bullet-}$
a	1.344(9)	1.37(2)	1.349(5)	1.407(10)	1.506(3)	1.423(4)
b	1.411(6)	1.404(15)	1.422(3)	1.378(13)	1.330(10)	1.378(4)
c	1.329(6)	1.335(14)	1.316(4)	1.336(7)	1.337(3)	1.312(4)
d	1.397(7)	1.39(2)	1.400(3)	1.399(8)	1.362(3)	1.389(3)

Table S3 Comparison of averaged bond lengths of reference compounds.

Bond	**Yb–bpym^{2-}–Yb**[10]	**Dy–bpym$^{\bullet-}$–Dy**[11]	**Tb–bpym$^{\bullet-}$–Tb**[11]
a	1.359(1)	1.401(7)	1.396(9)
b	1.422(10)	1.383(6)	1.376(8)
c	1.313(11)	1.340(8)	1.344(10)
d	1.406(13)	1.377(9)	1.381(10)

Electrochemistry data

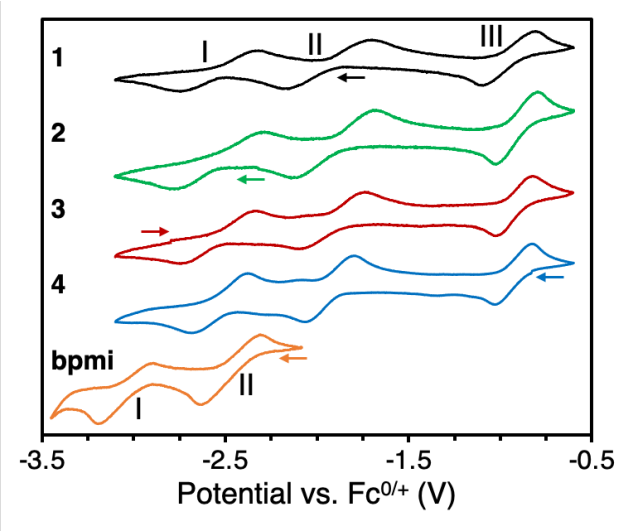

Figure S17 Cyclic voltammograms of crystals of complexes **1**-**4** and 2,2'-bipyrimidine (bpym) in THF/0.06 M $[NBu_4][BPh_4]$ at a 50 mV/s scan rate versus $Fc^{0/+}$ using a Pt^0 disk as a working electrode (arrow indicates scan direction).

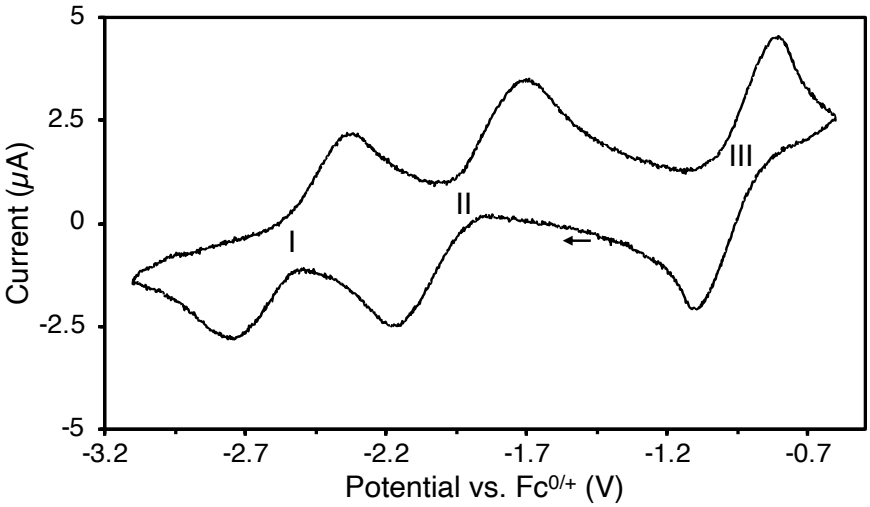

Figure S18 Cyclic voltammogram of crystals of **1** in THF/0.06 M $[NBu_4][BPh_4]$ at a 50 mV/s scan rate versus $Fc^{0/+}$ using a Pt^0 disk as a working electrode (arrow indicates scan direction).

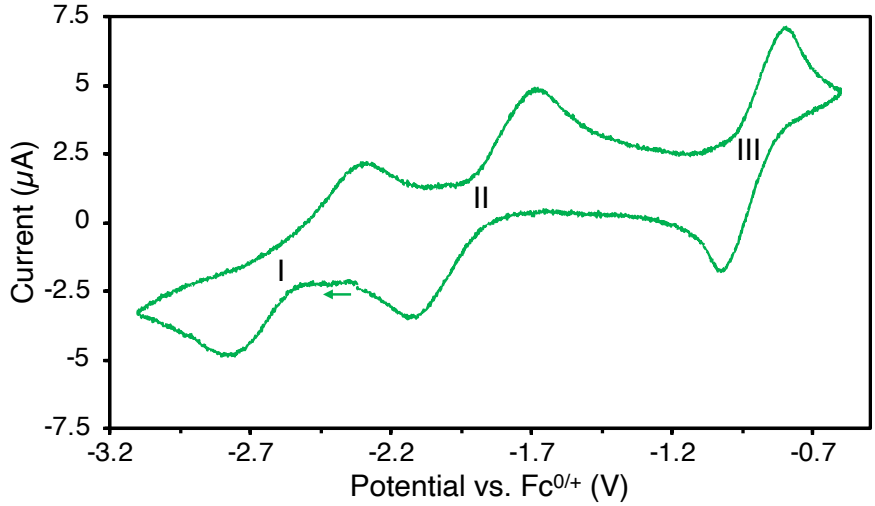

Figure S19 Cyclic voltammogram of crystals of **2** in THF/0.06 M $[NBu_4][BPh_4]$ at a 50 mV/s scan rate versus $Fc^{0/+}$ using a Pt^0 disk as a working electrode (arrow indicates scan direction).

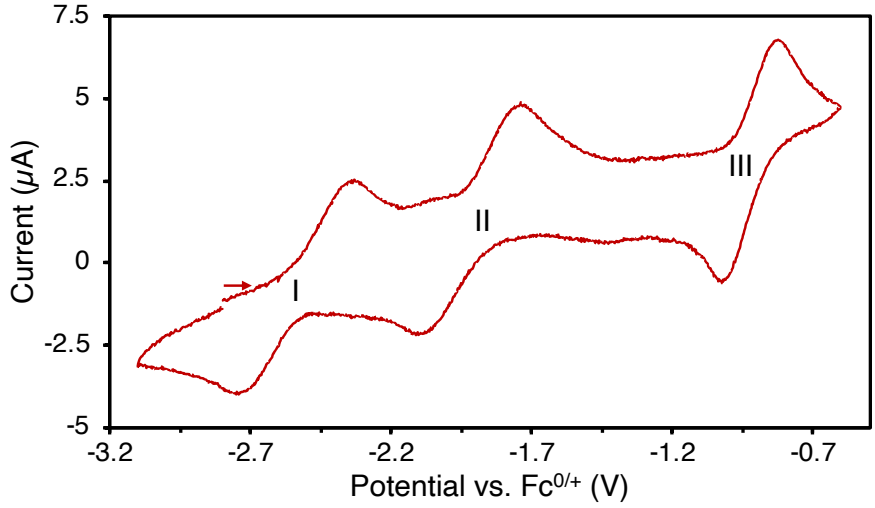

Figure S20 Cyclic voltammogram of crystals of **3** in THF/0.06 M $[NBu_4][BPh_4]$ at a 50 mV/s scan rate versus $Fc^{0/+}$ using a Pt^0 disk as a working electrode (arrow indicates scan direction).

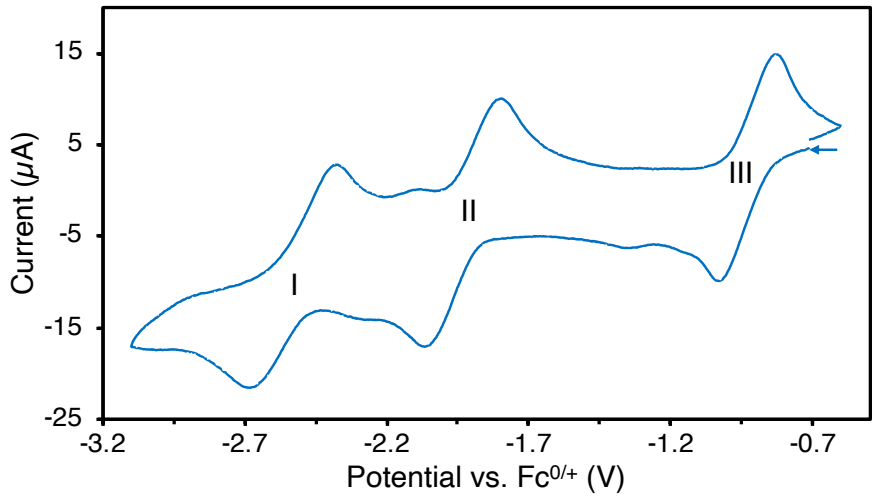

Figure S21 Cyclic voltammogram of crystals of **4** in THF/0.06 M $[NBu_4][BPh_4]$ at a 50 mV/s scan rate versus $Fc^{0/+}$ using a Pt^0 disk as a working electrode (arrow indicates scan direction).

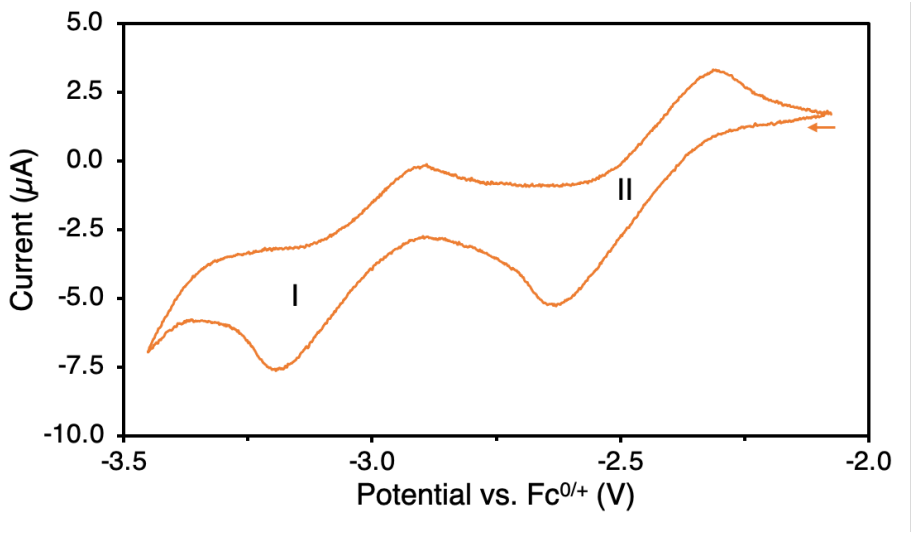

Figure S22 Cyclic voltammogram of 2,2'-bipyrimidine in THF/0.06 M $[NBu_4][BPh_4]$ at a 50 mV/s scan rate versus $Fc^{0/+}$ using a Pt^0 disk as a working electrode (arrow indicates scan direction).

Table S4 Potentials of cathodic and anodic waves observed in the cyclic voltammograms of complexes **1-4** and 2,2'-bipyrimidine (bpym).

Wave	**I**		**II**		**III**	
Complex	E_{pc} (V)	E_{pa} (V)	E_{pc} (V)	E_{pa} (V)	E_{pc} (V)	E_{pa} (V)
1	–2.75	–2.34	–2.19	–1.69	–1.10	–0.80
2	–2.74	–2.32	–2.10	–1.72	–1.03	–0.82
3	–2.76	–2.29	–2.14	–1.68	–1.04	–0.80
4	–2.68	–2.37	–2.06	–1.80	–1.03	–0.83
bpym	–3.19	–2.89	–2.63	–2.31		

DC magnetic data

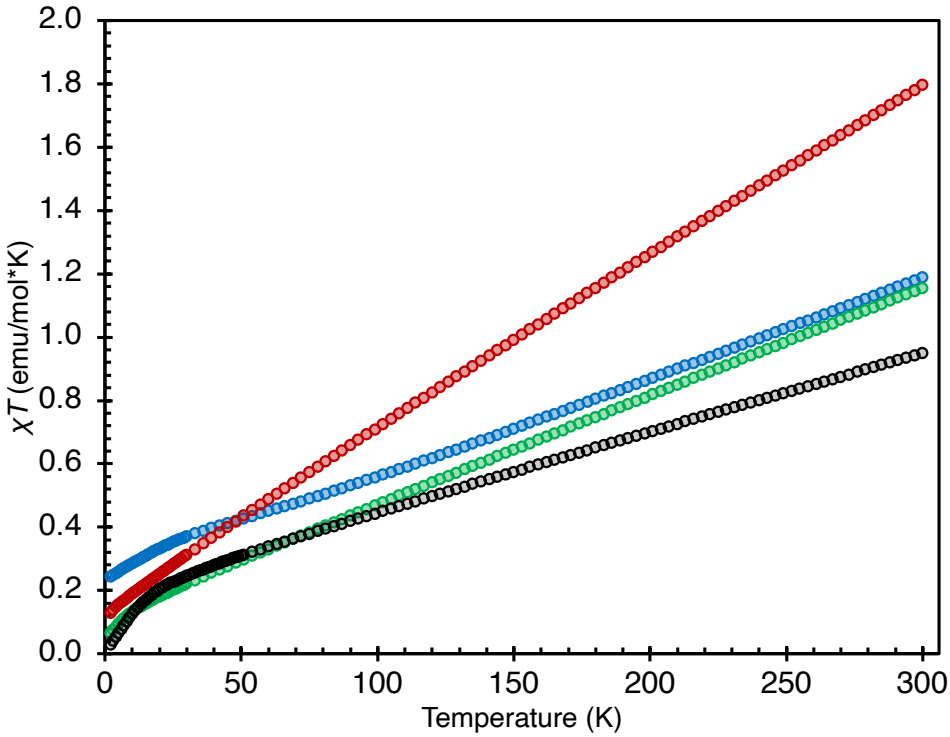

Figure S23 χT(T) product overlay of complexes **1-4** up to 300 K (black, **1**; green, **2**; red, **3**; blue, **4**).

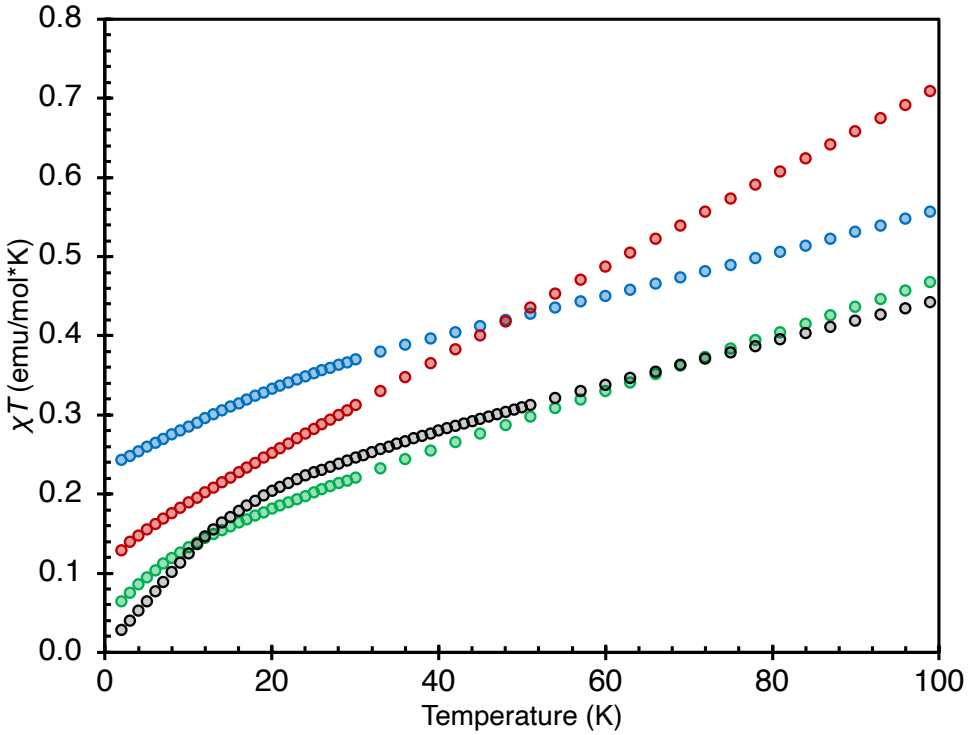

Figure S24 χT(T) product overlay of complexes **1-4** up to 100 K (black, **1**; green, **2**; red, **3**; blue, **4**).

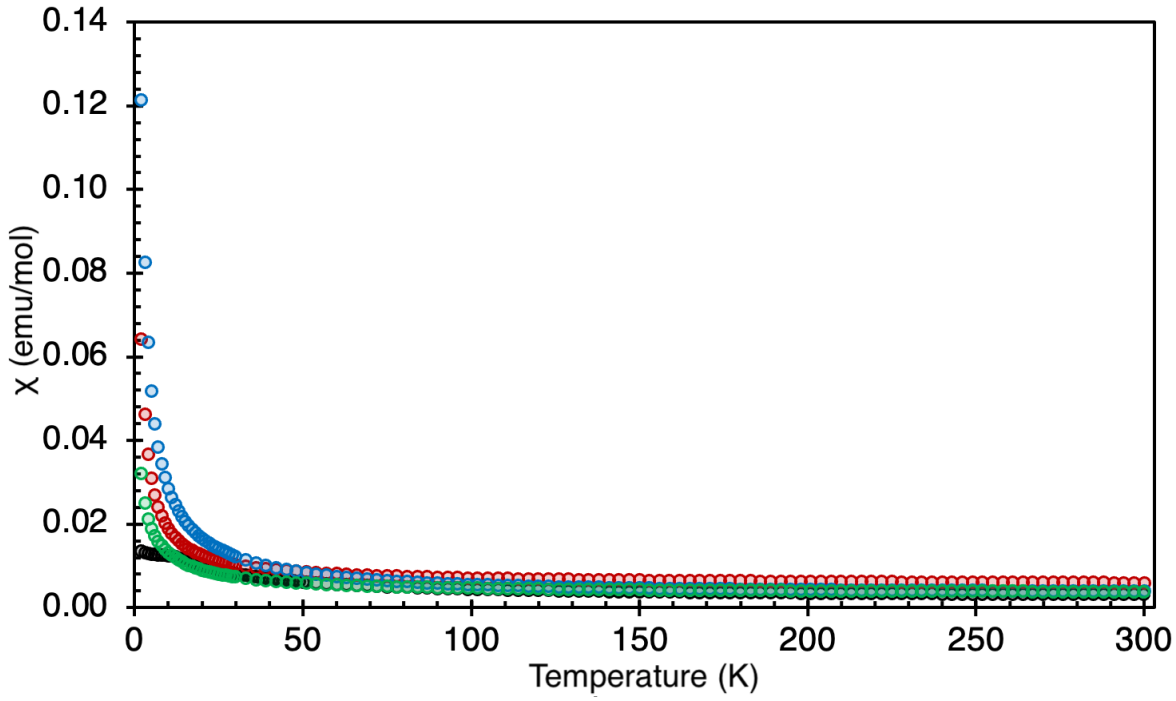

Figure S25 Chi(T) product overlays of complexes **1**-**4** up to 300 K (black, **1**; green, **2**; red, **3**; blue, **4**).

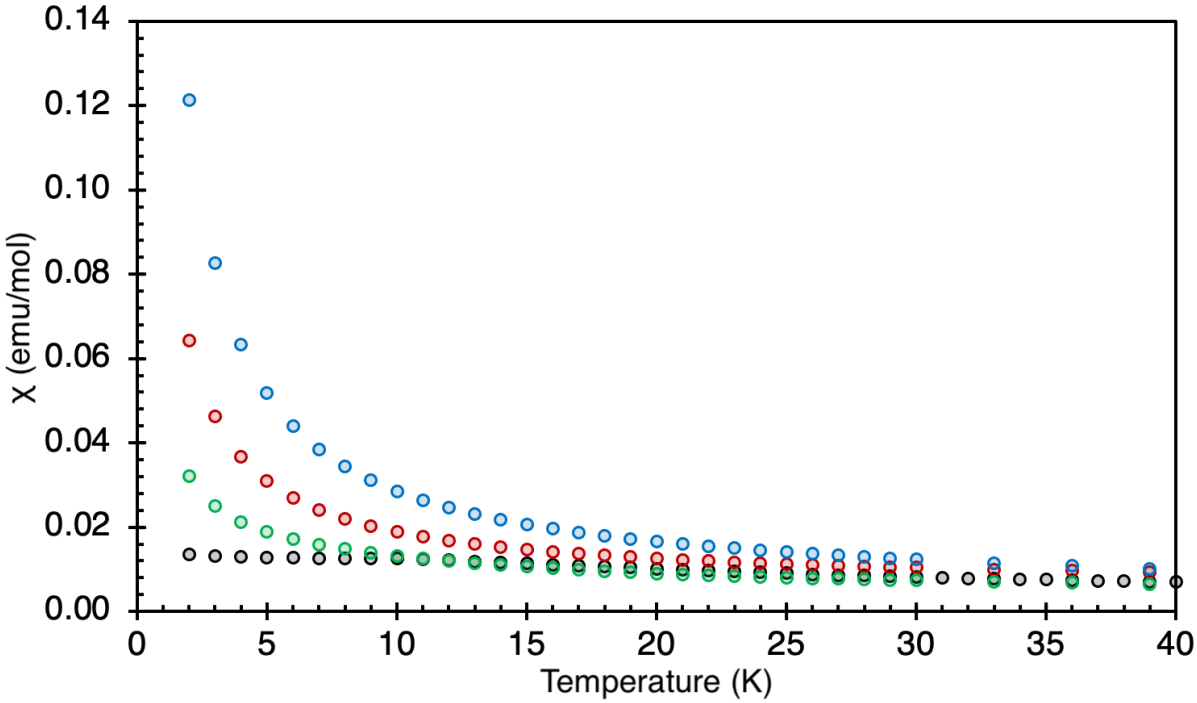

Figure S26 Chi(T) product overlays of complexes **1**-**4** up to 40 K (black, **1**; green, **2**; red, **3**; blue, **4**).

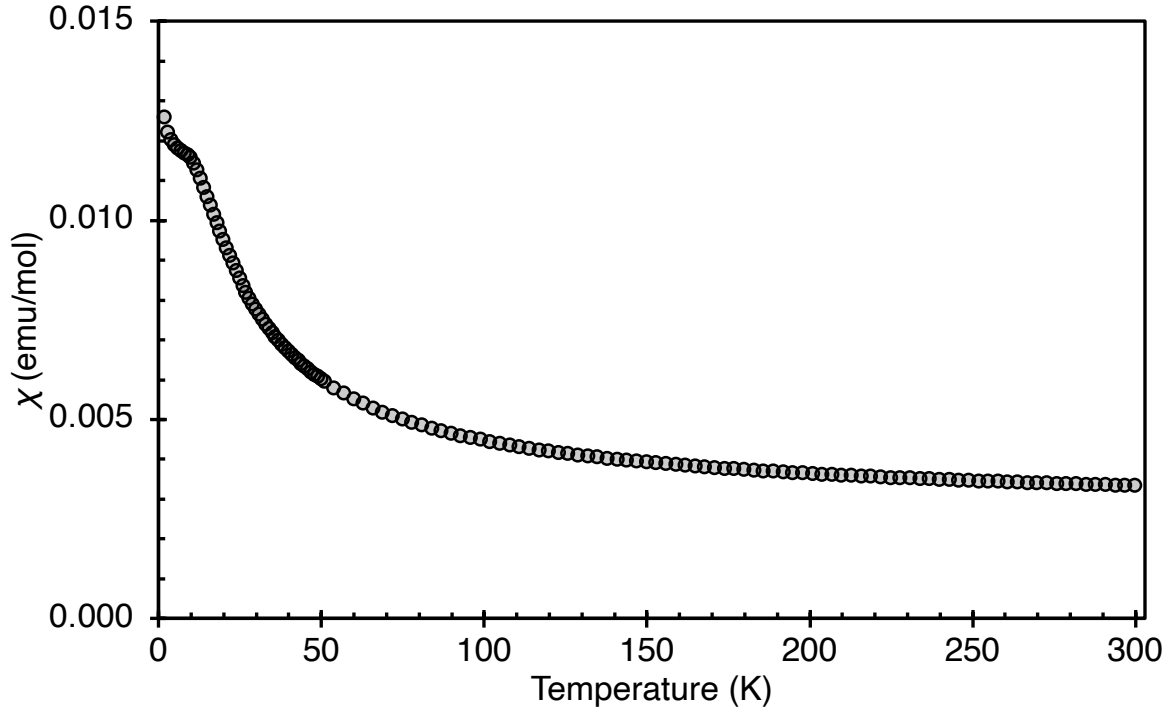

Figure S27 Molar magnetic susceptibility per uranium center versus temperature for complex **1**, measured under applied field of 0.1 T.

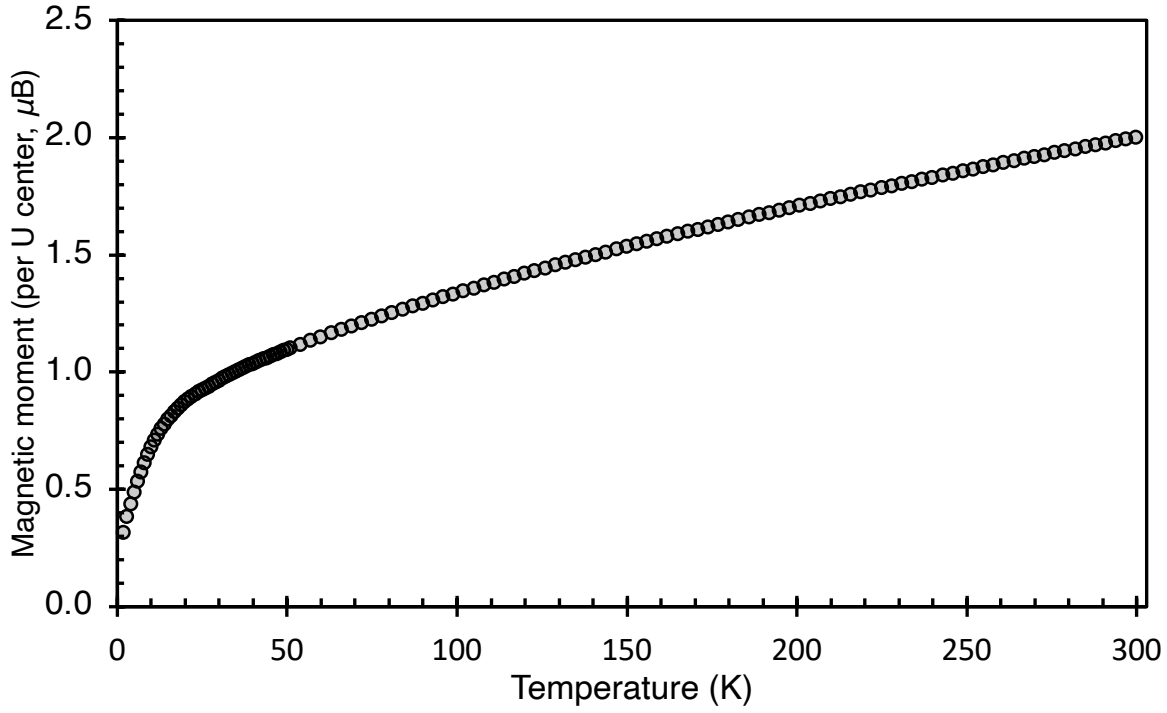

Figure S28 Magnetic moment per uranium center versus temperature for complex **1**, measured under applied field of 0.1 T.

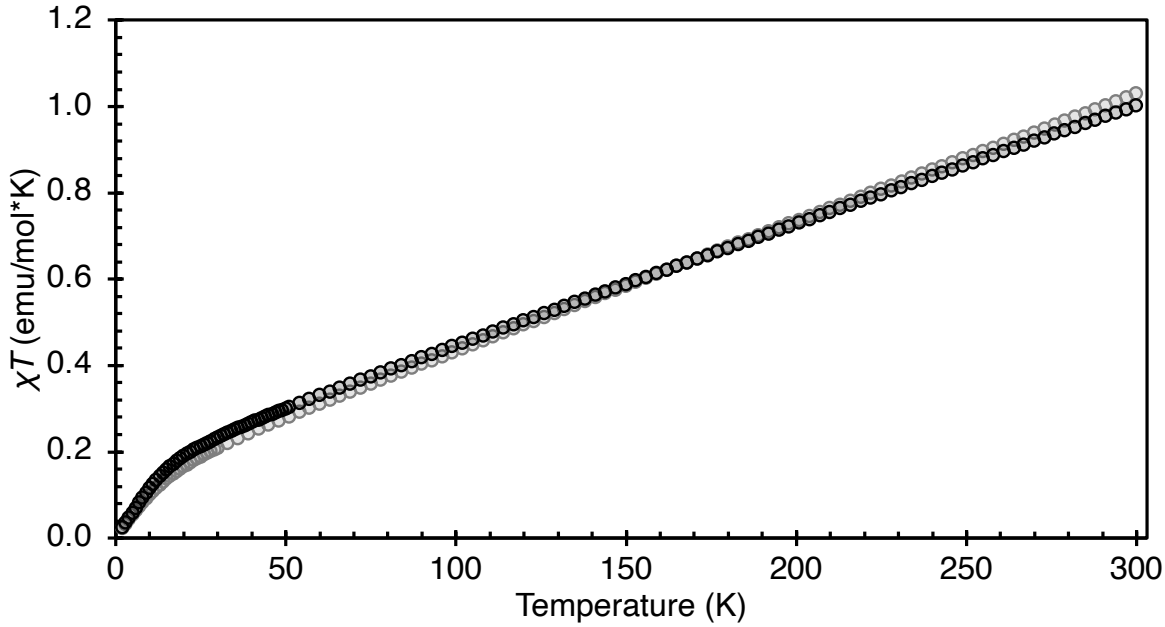

Figure S29 Temperature-dependent magnetization data for two independently synthesized samples of **1**, shown as overlayed χT(T) products.

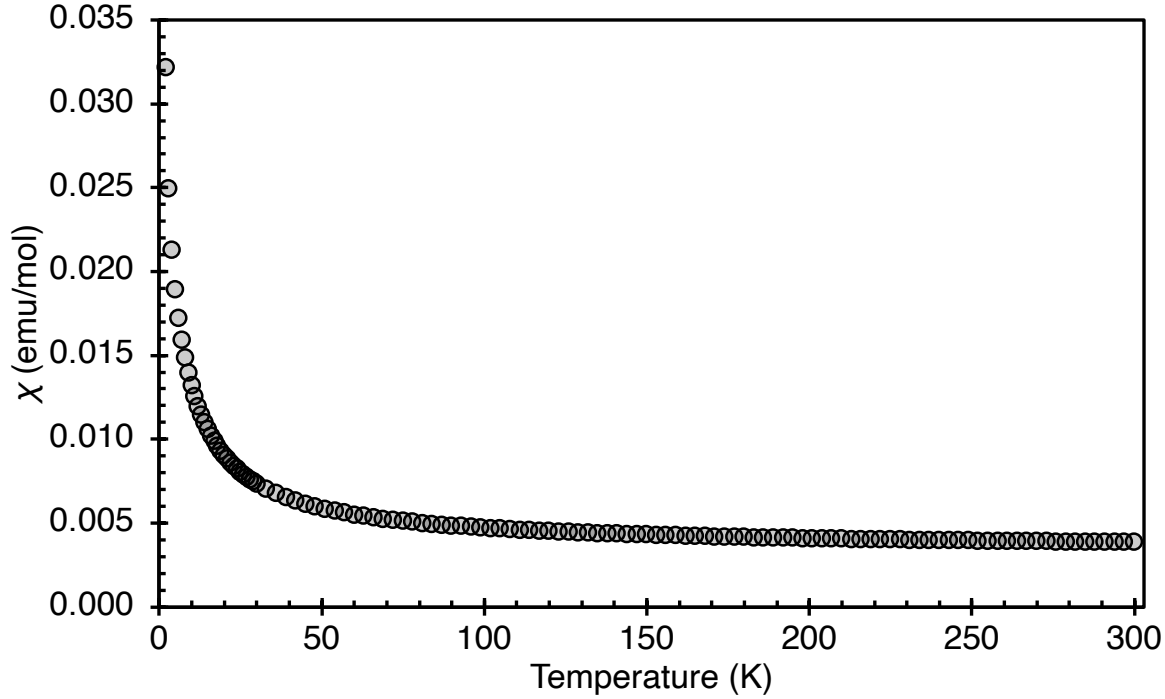

Figure S30 Molar magnetic susceptibility per uranium center versus temperature for complex **2**, measured under applied field of 0.1 T.

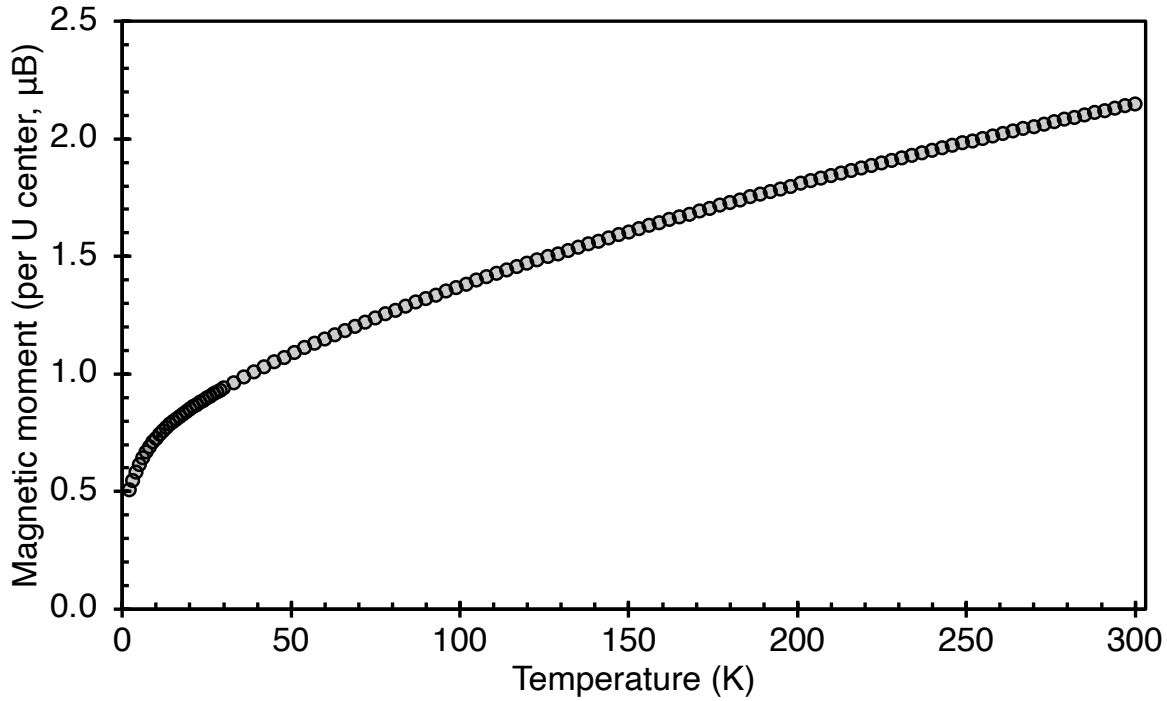

Figure S31 Magnetic moment per uranium center versus temperature for complex **2**, measured under applied field of 0.1 T.

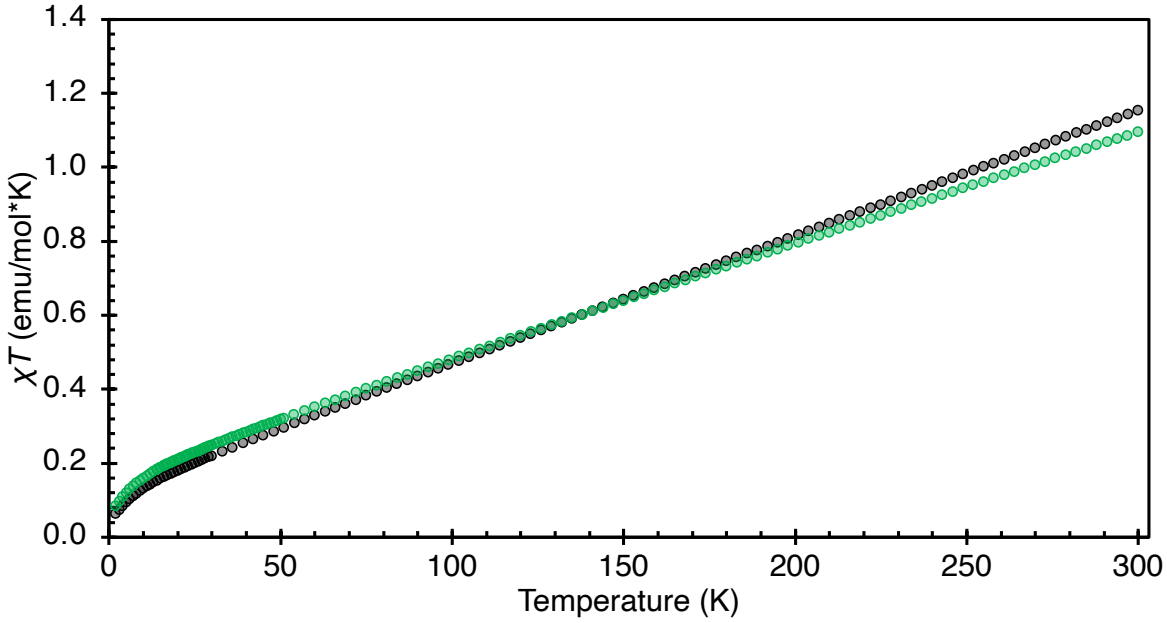

Figure S32 Temperature-dependent magnetization data for two independently synthesized samples of **2**, shown as overlayed χT(T) products.

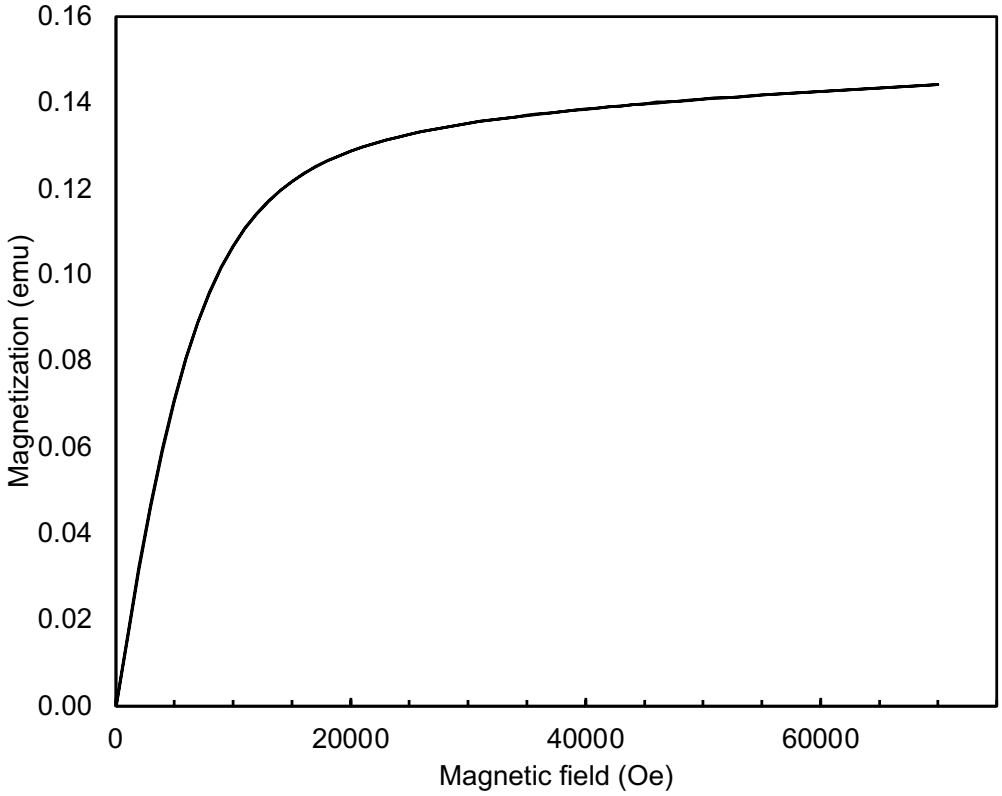

Figure S33 M(H) curve (hysteresis loop) for the complex **2** at 1.8 K.

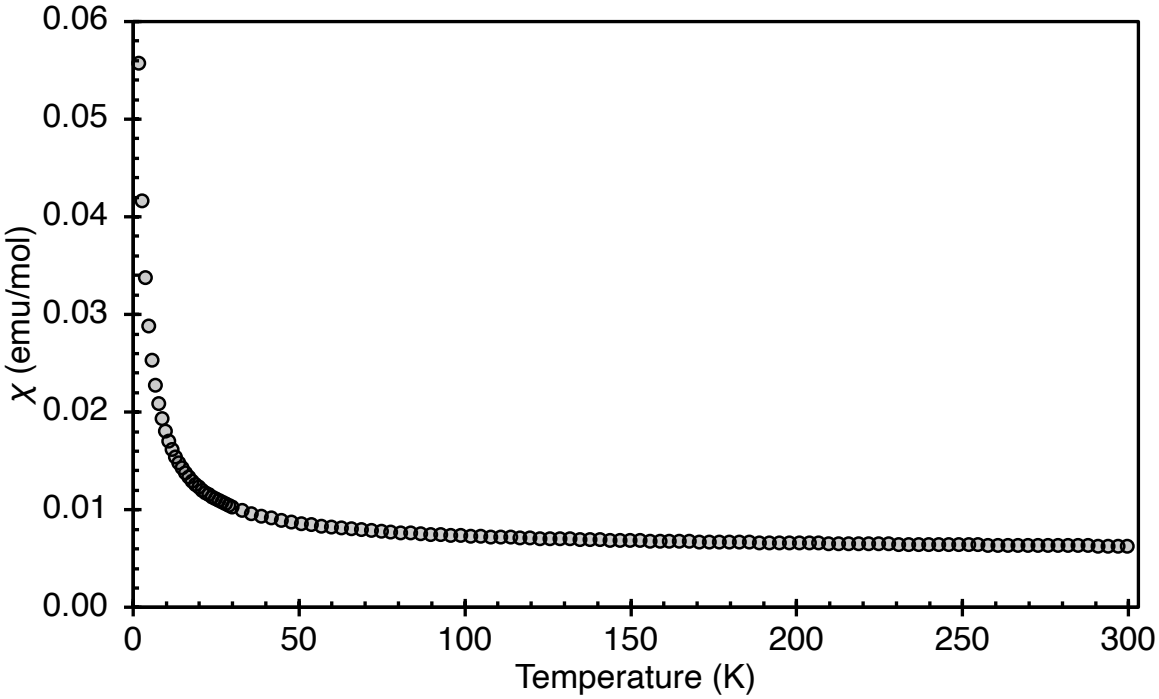

Figure S34 Magnetic moment per uranium center versus temperature for complex **3**, measured under applied field of 0.1 T.

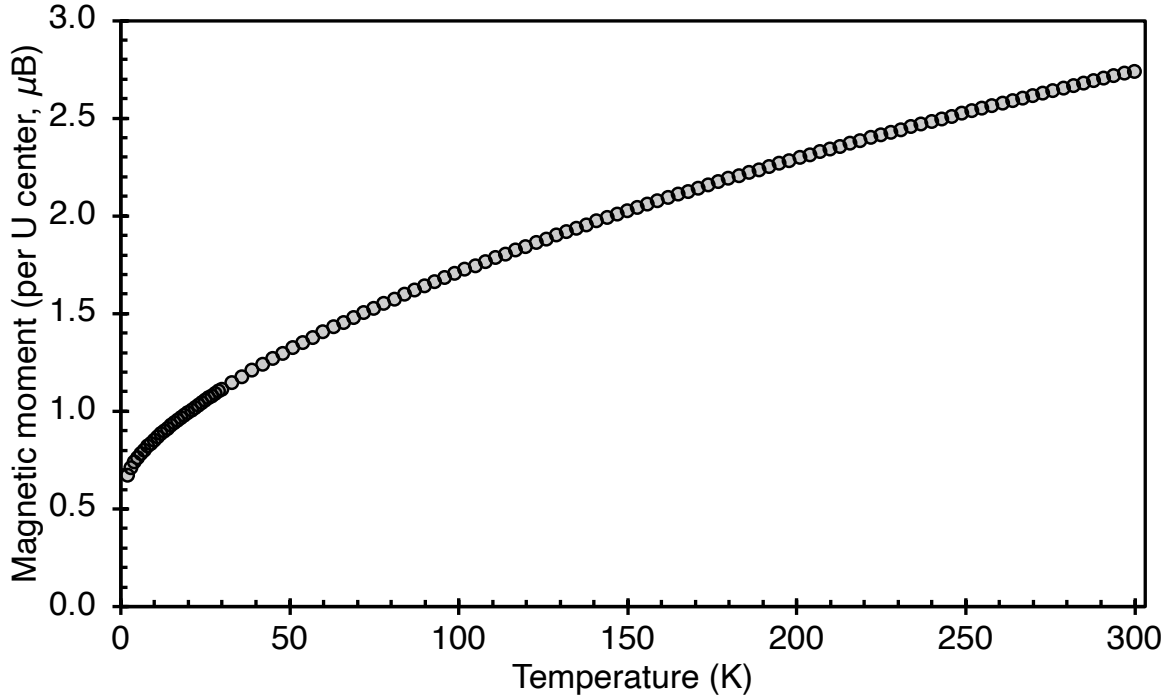

Figure S35 Magnetic moment per uranium center versus temperature for complex **3**, measured under applied field of 0.1 T.

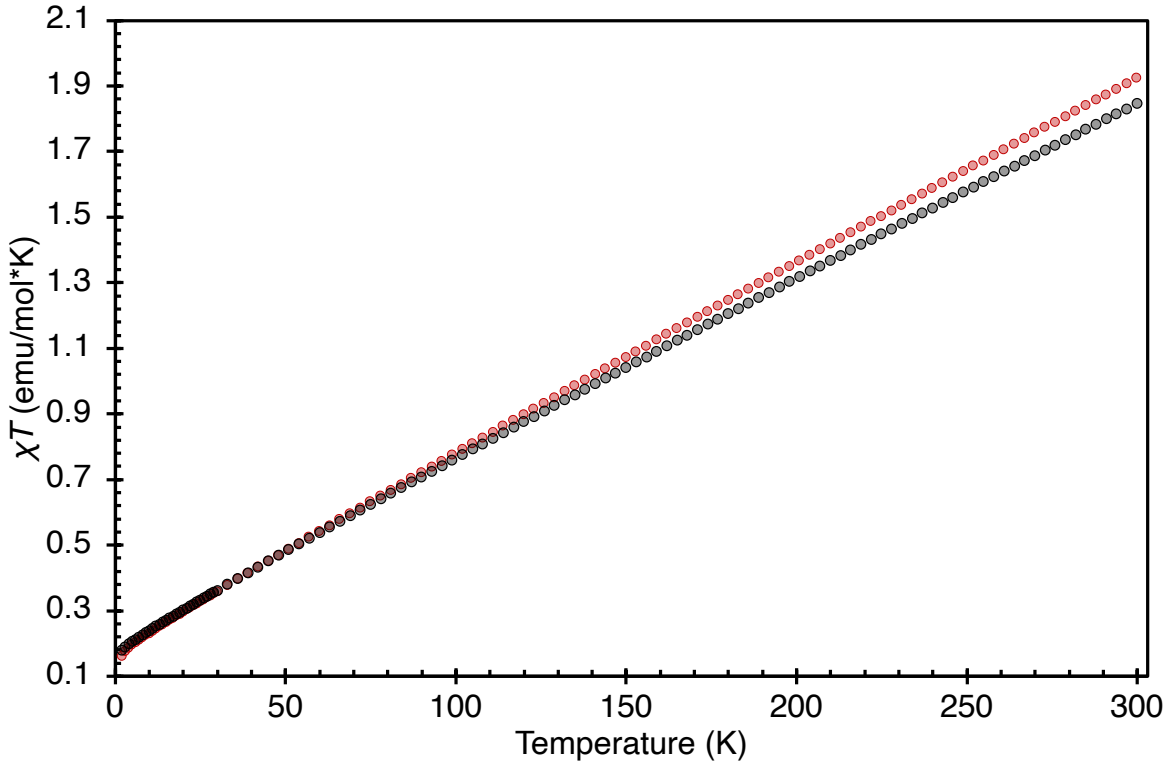

Figure S36 Temperature-dependent magnetization data for two independently synthesized samples of **3**, shown as overlayed χT(T) products.

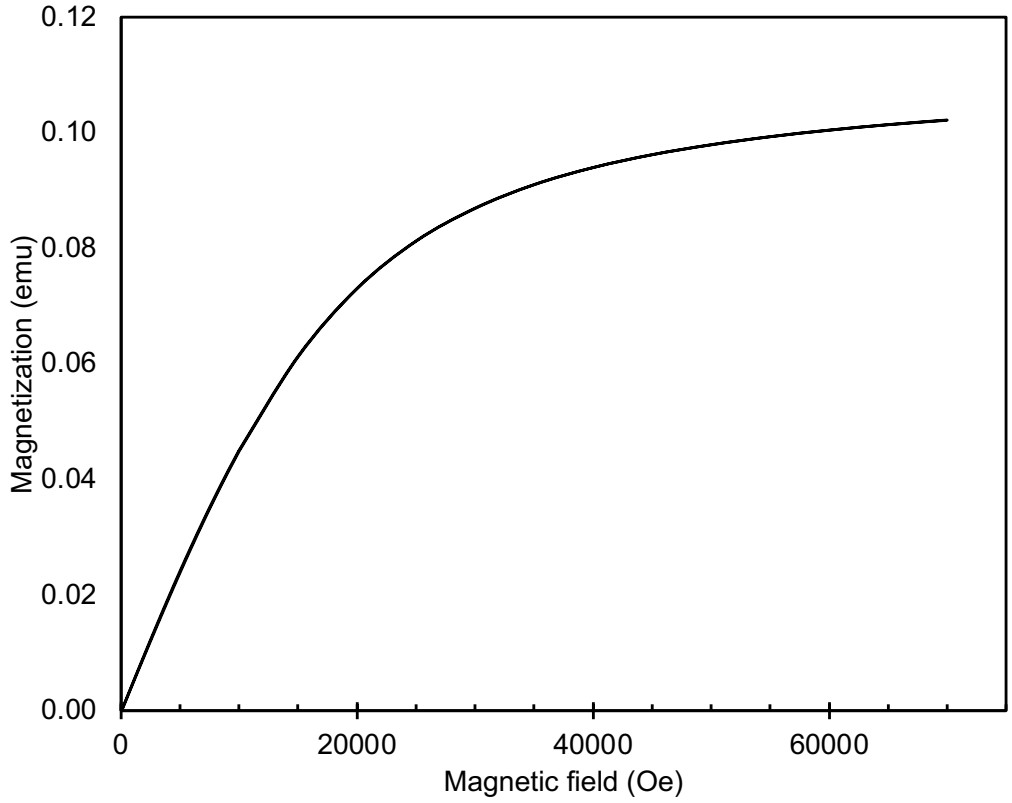

Figure S37 M(H) curve (hysteresis loop) for the complex **3** at 1.8 K.

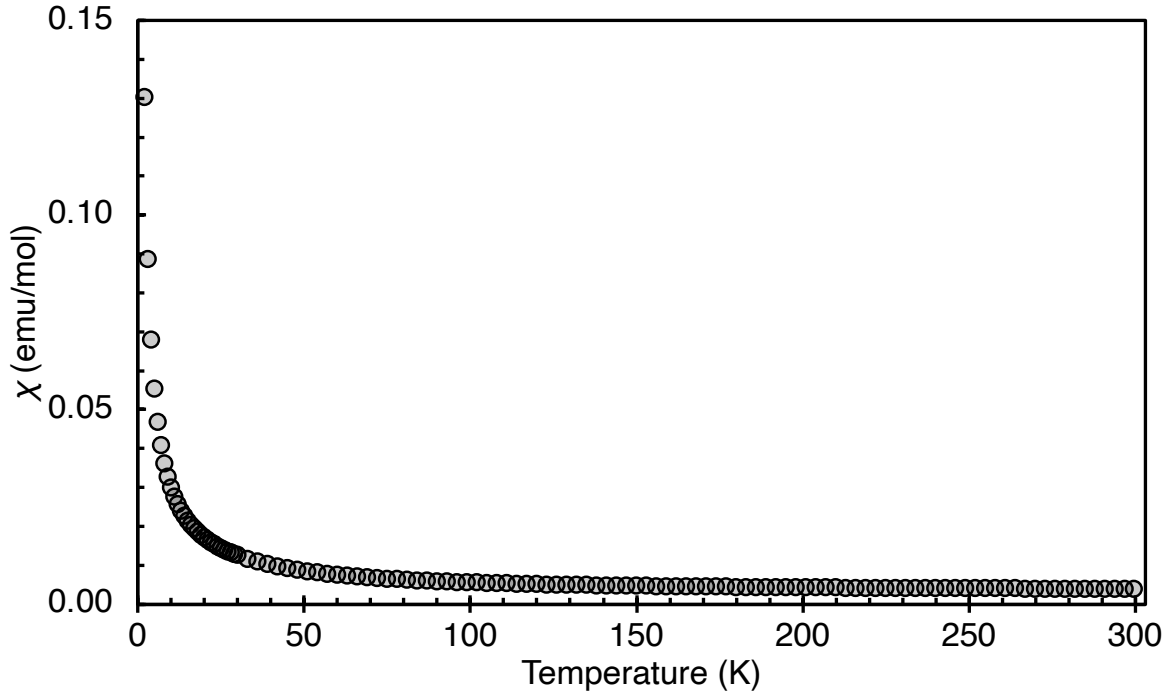

Figure S38 Molar magnetic susceptibility versus temperature for complex **4**, measured under applied field of 0.1 T.

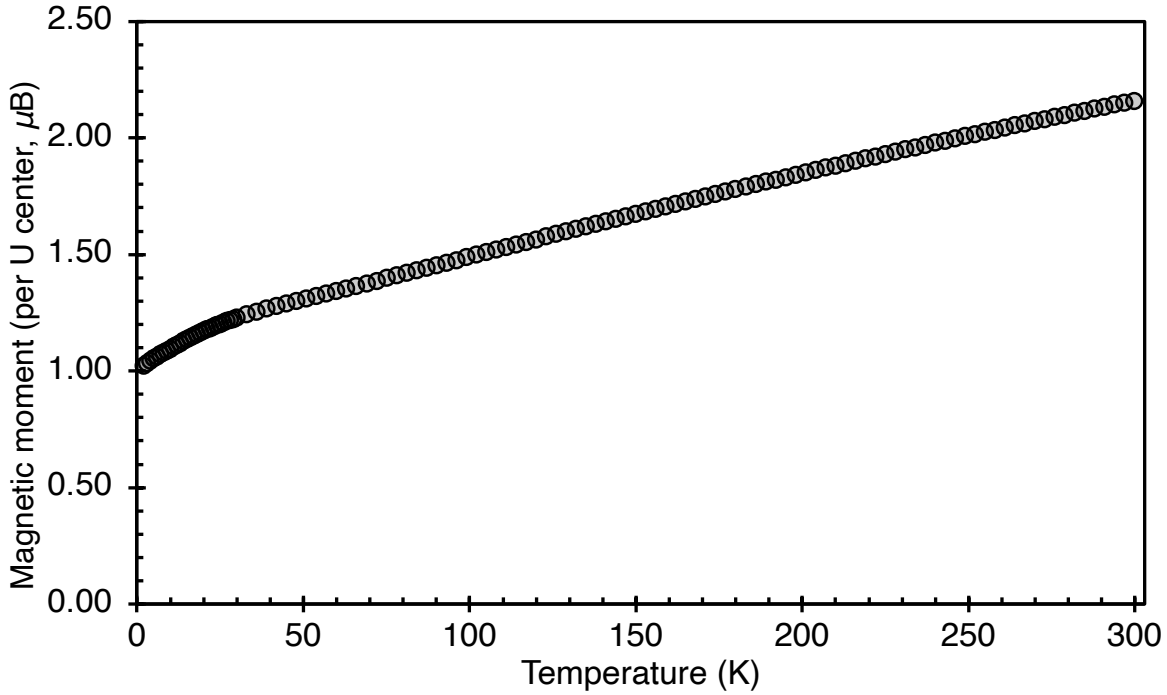

Figure S39 Magnetic moment per uranium center versus temperature for complex **4**, measured under applied field of 0.1 T.

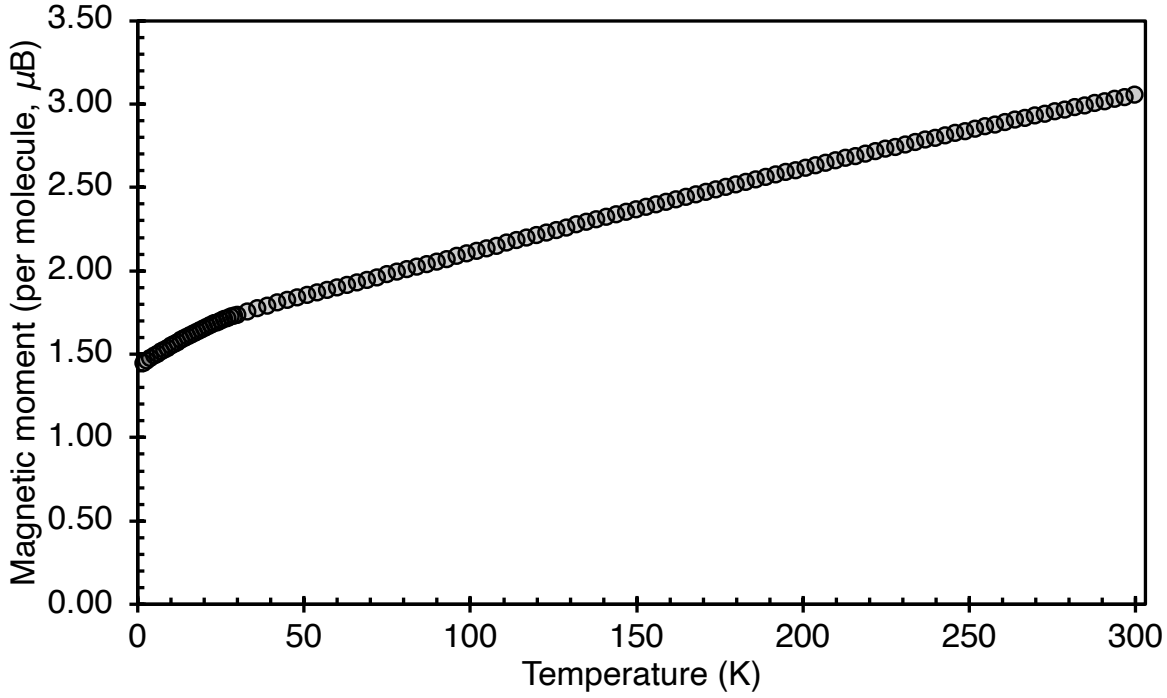

Figure S40 Magnetic moment per molecule versus temperature for complex **4**, measured under applied field of 0.1 T.

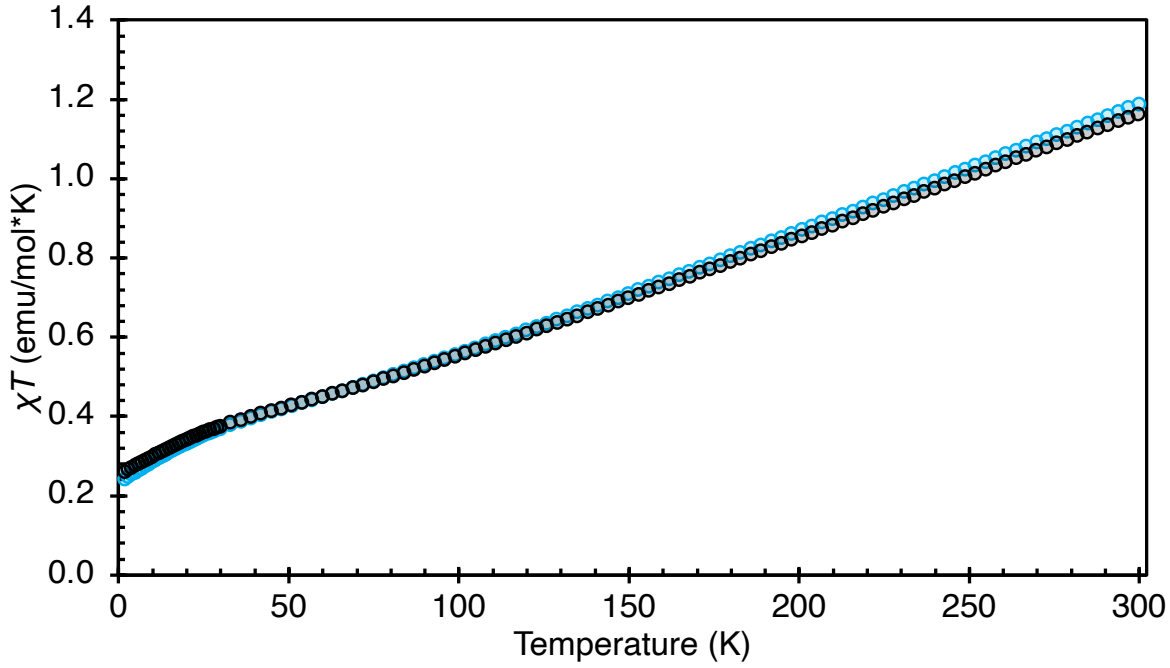

Figure S41 Temperature-dependent magnetization data for two independently synthesized samples of **4**, shown as overlayed χT(T) products.

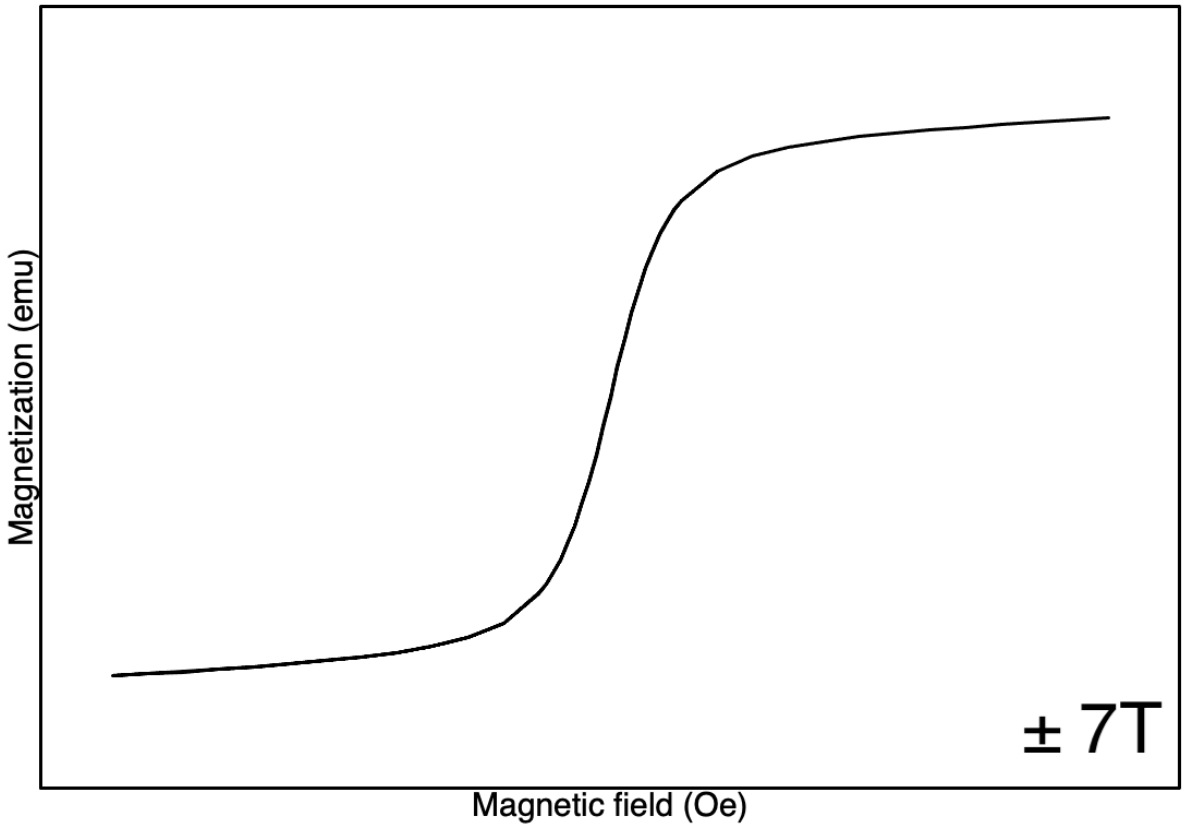

Figure S42 M(H) curve (hysteresis loop) for the complex **4** at 1.8 K.

EPR measurements

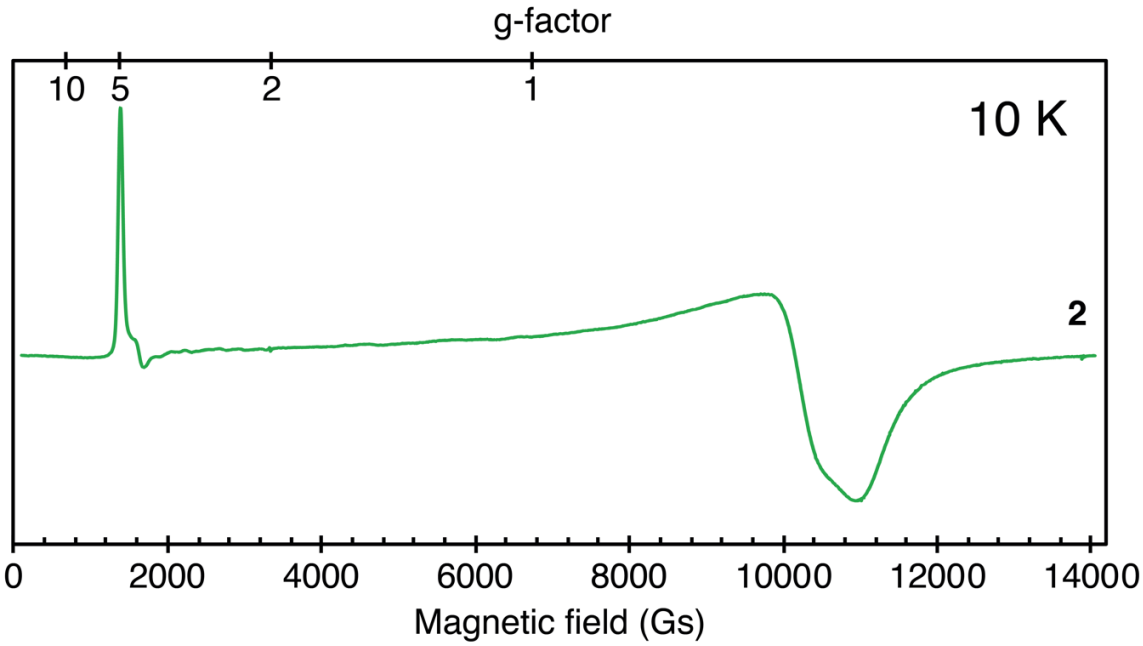

Figure S43 Solid-state EPR spectrum of complex **2**, recorded at 10 K.

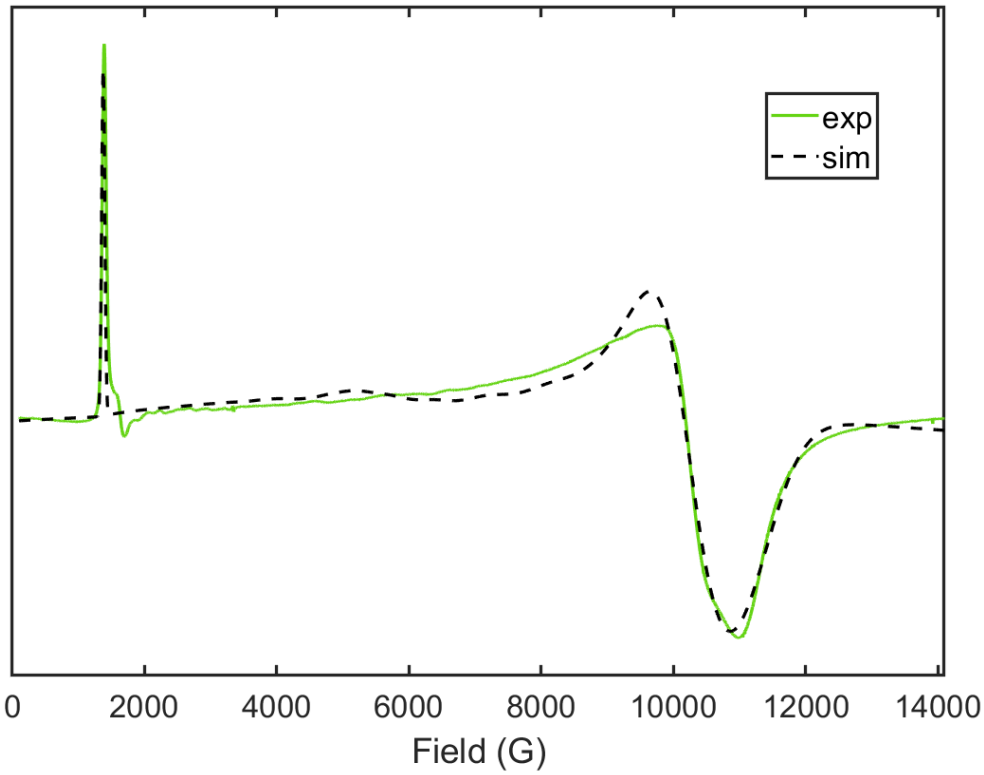

Figure S44 Modelling of solid-state EPR spectrum of complex **2** at 10 K, preformed in EasySpin package. Modelling parameters are: g = [4.88; 0.652; 0.607], H_{strain} = [380; 850; 1050]

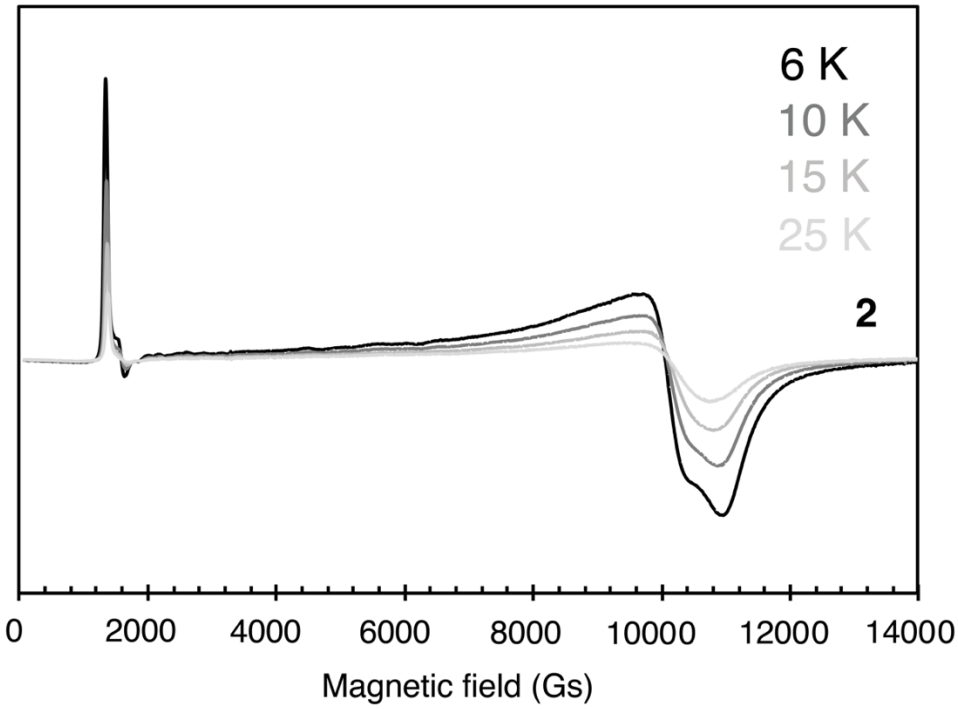

Figure S45 Variable temperature solid-state EPR spectra of complex 2.

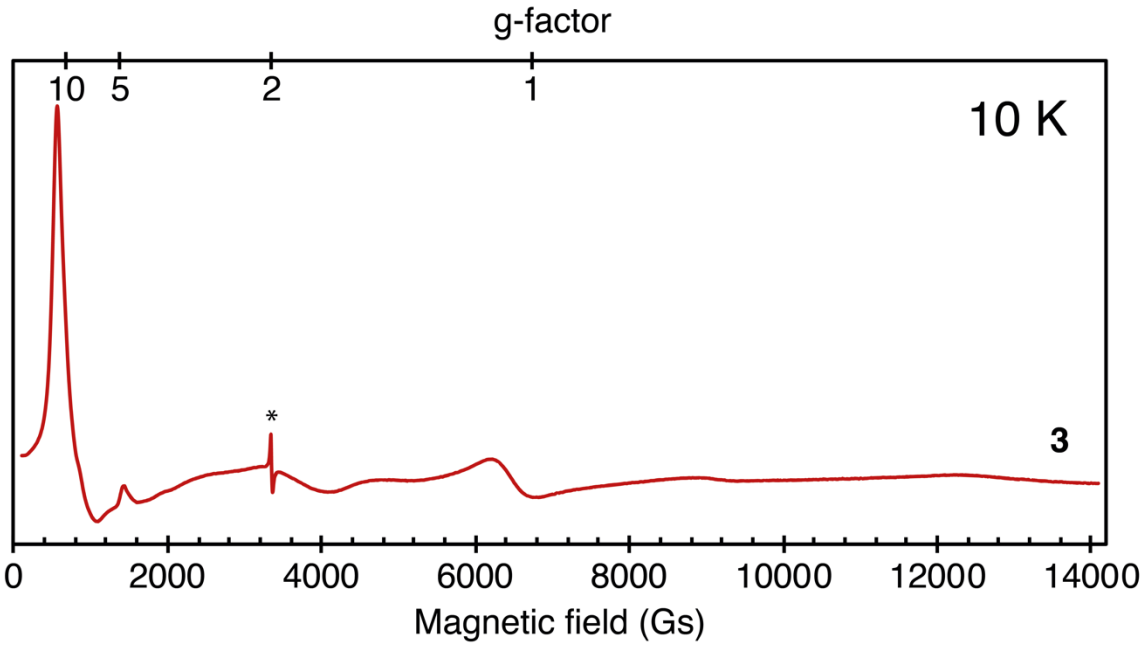

Figure S46 Solid-state EPR spectrum of complex **3**, recorded at 10 K.

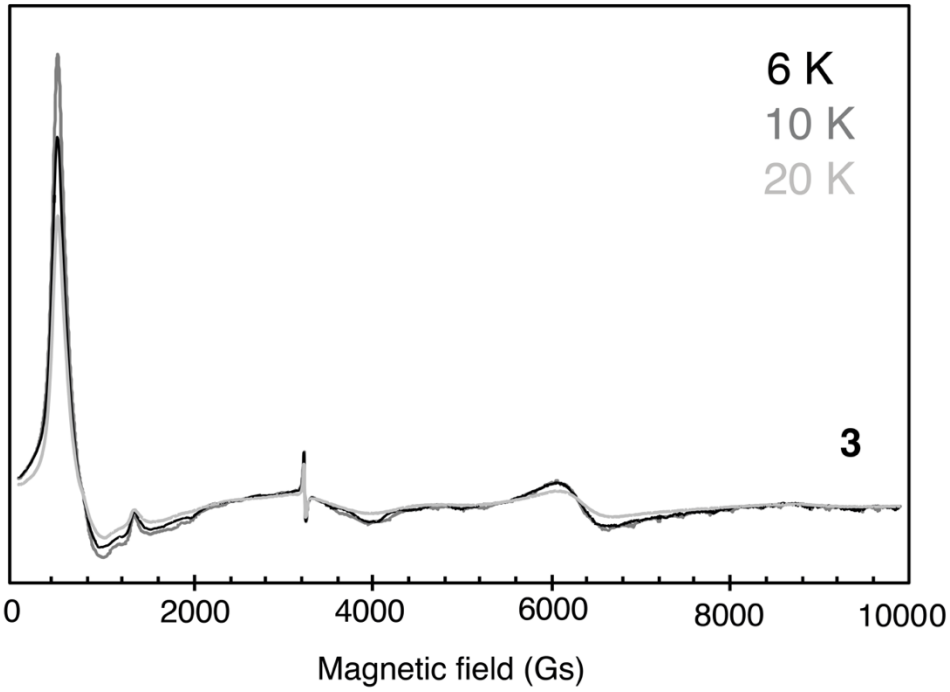

Figure S47 Variable temperature solid-state EPR spectra of complex 3.

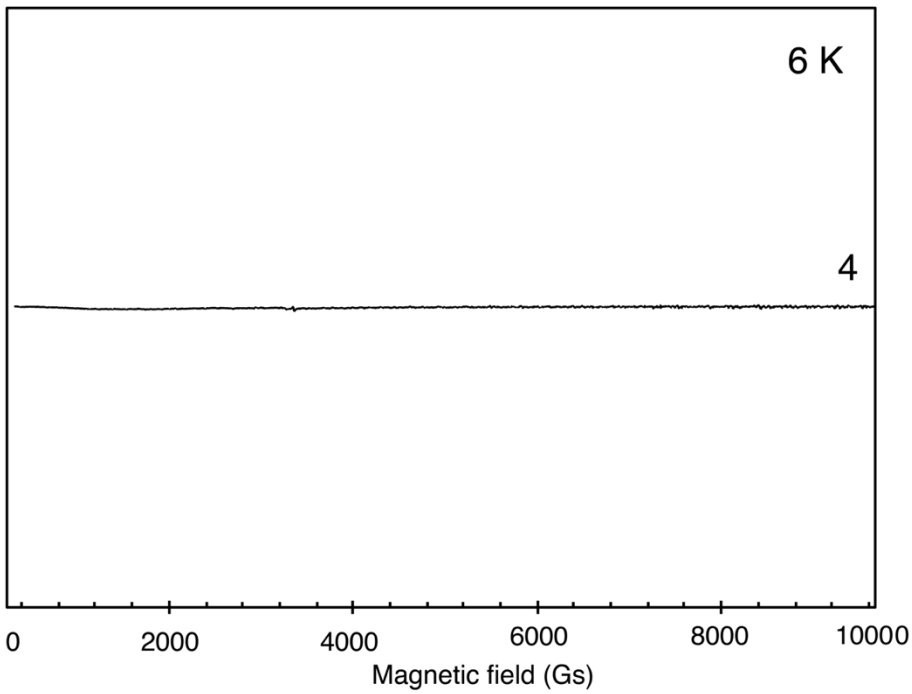

Figure S48 Solid-state EPR spectra of radical-bridged complex **4** at 6 K (no signal above noise level).

AC magnetic data

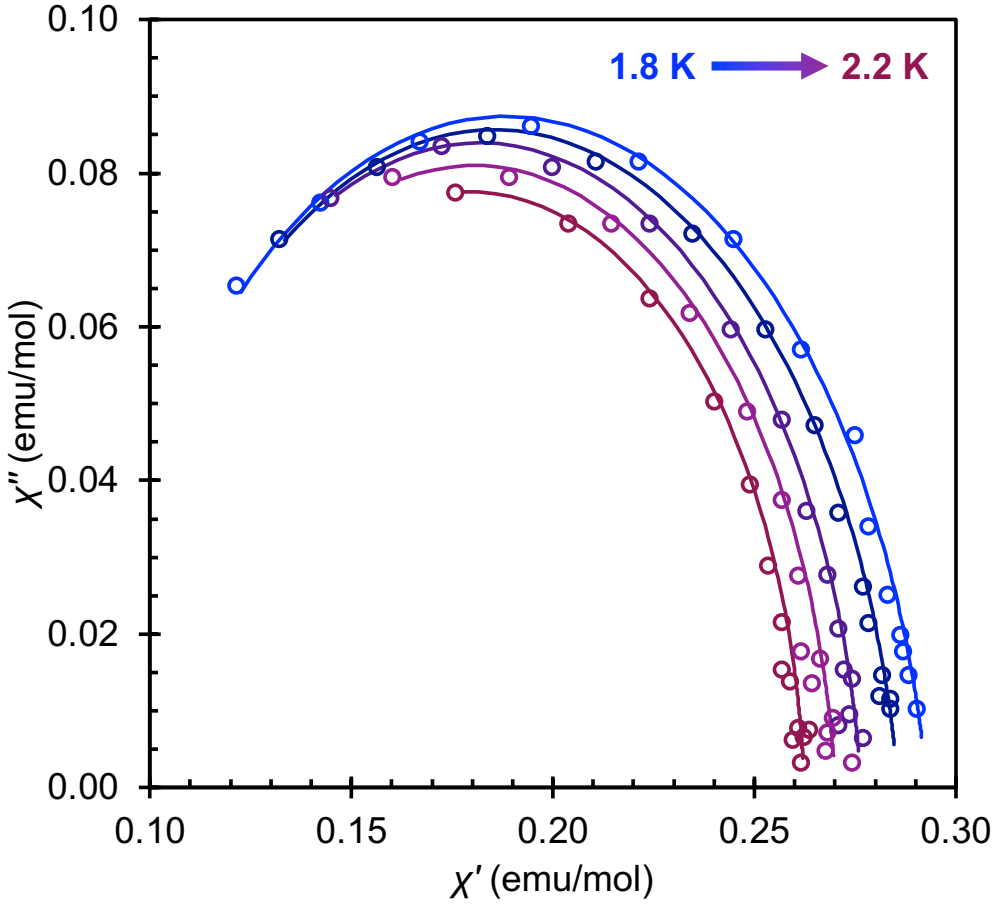

Figure S49 Argand (Cole-Cole) plot (points) for **2**, fitted with generalised Debye model (lines) in the temperature range 1.8-2.2 K under 0.2 T DC field.

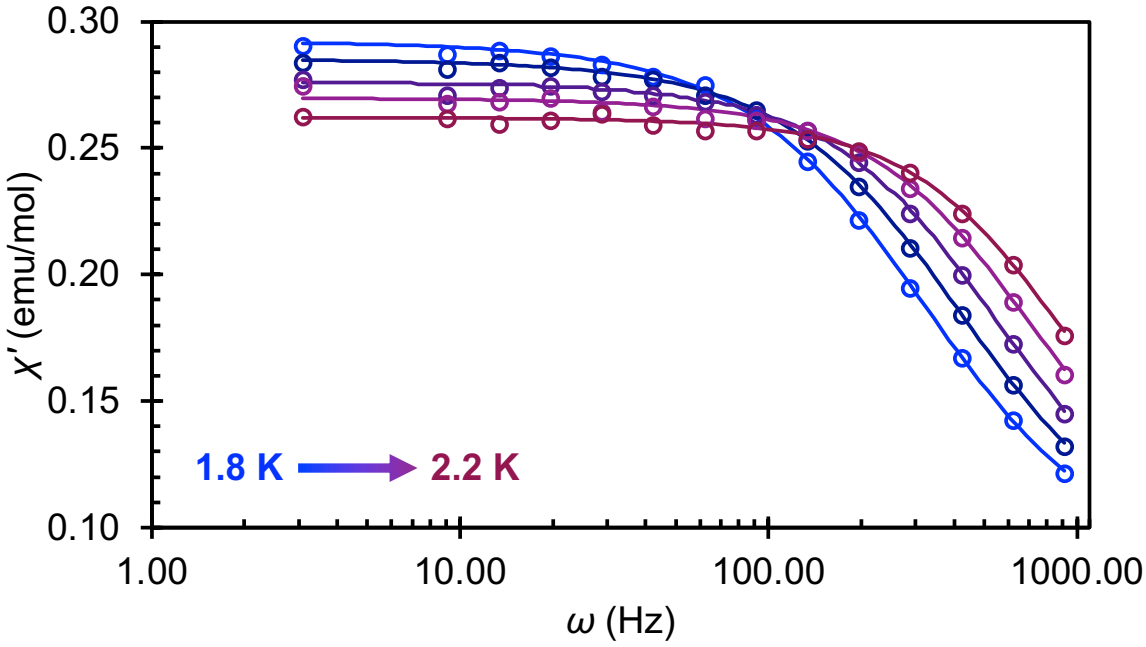

Figure S50 In-phase (χ') AC susceptibility for **2**, fitted with generalised Debye model in the temperature range 1.8-2.2 K under 0.2 T DC field.

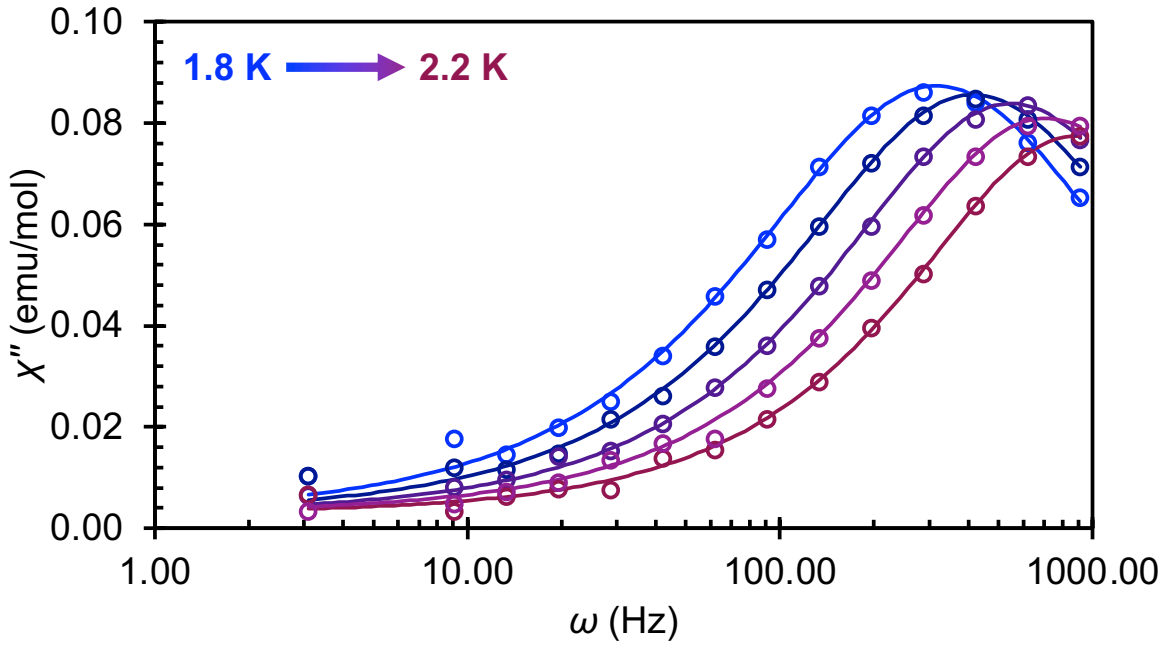

Figure S51 Out-of-phase (χ'') AC susceptibility for **2**, fitted with generalised Debye model in the temperature range 1.8-2.2 K under 0.2 T DC field.

Table S5 Table of extracted constant temperature susceptibility (χT), adiabatic susceptibility (χS), parameter gauging the width of distribution of relaxation times (α) and relaxation time (τ) at each individual temperature, for compound **2** under an applied field of 0.2 T

T (K)	χT (emu/mol)	χS (emu/mol)	α	τ (s)
1.80	0.29	0.08	0.13	0.001072(9)
1.90	0.29	0.09	0.12	0.000782(6)
2.00	0.28	0.09	0.10	0.000544(5)
2.10	0.27	0.09	0.09	0.000404(8)
2.20	0.26	0.10	0.06	0.000293(6)

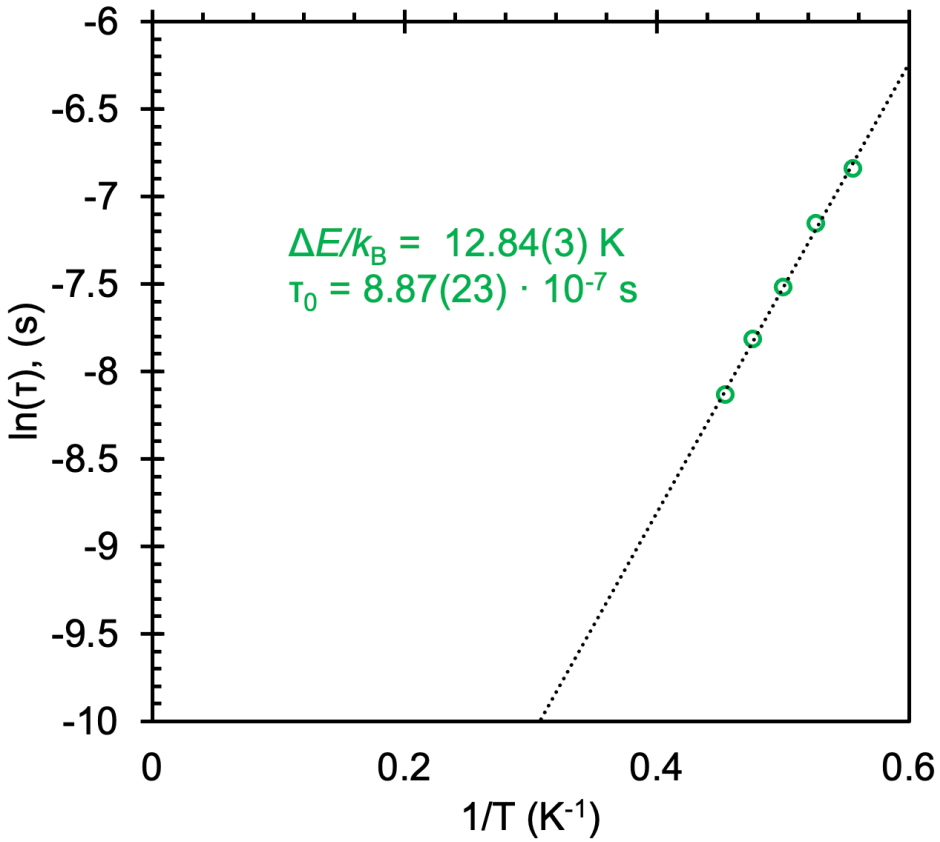

Figure S52 Arrhenius plot of **2** in the temperature region 1.8-2.2 K under 0.2 T DC field, with the obtained parameters of $\Delta E/k_B$ = 12.84(3) K, τ_0 = 8.87(23) · 10^{-7} s. The fit is extended to show linearity.

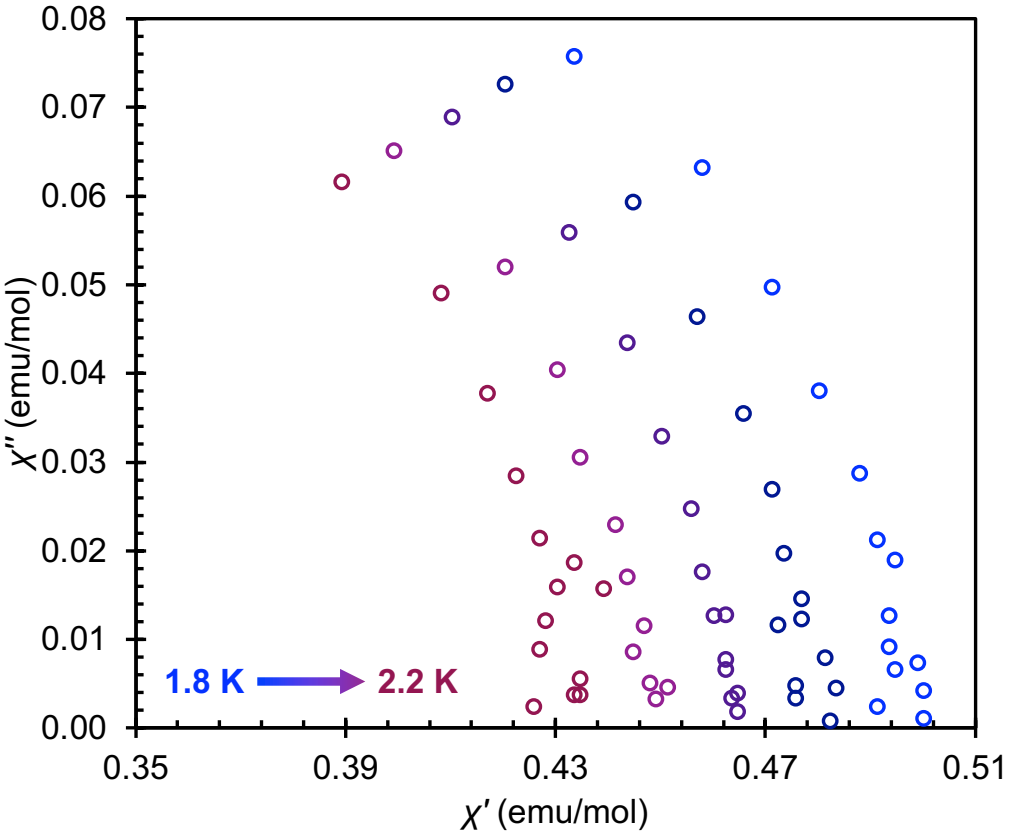

Figure S53 Argand (Cole-Cole) plot for 3 (no visible maximum).

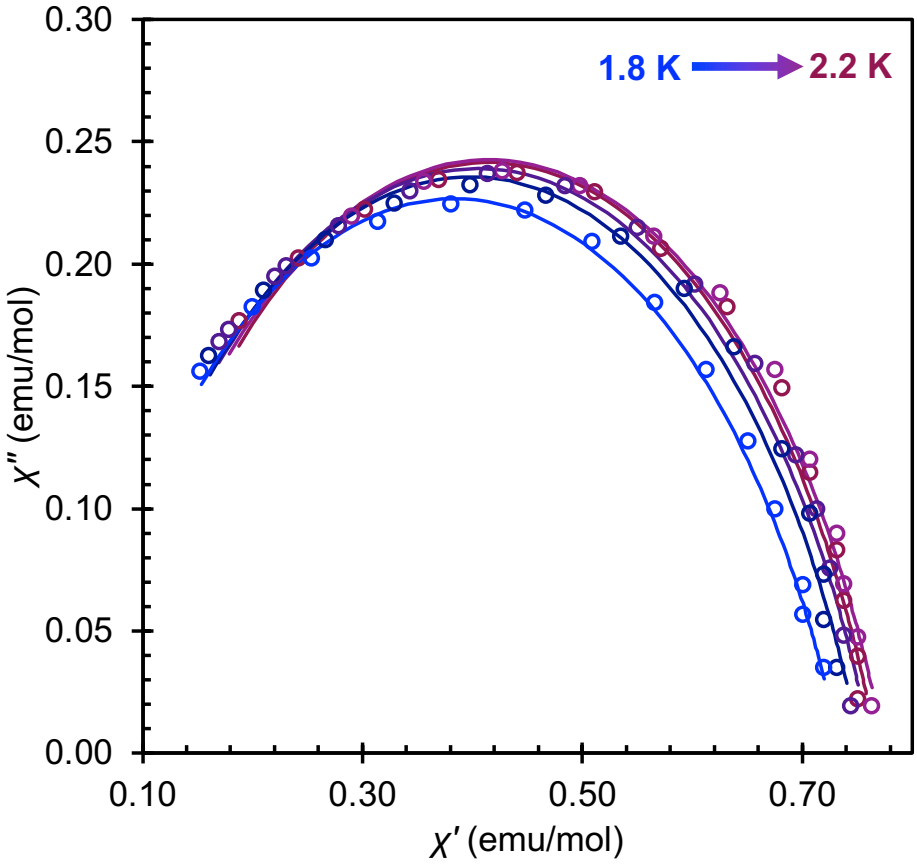

Figure S54 Argand (Cole-Cole) plot (points) for **4**, fitted with generalised Debye model (lines) in the temperature range 1.8-2.2 K under 0.2 T DC field.

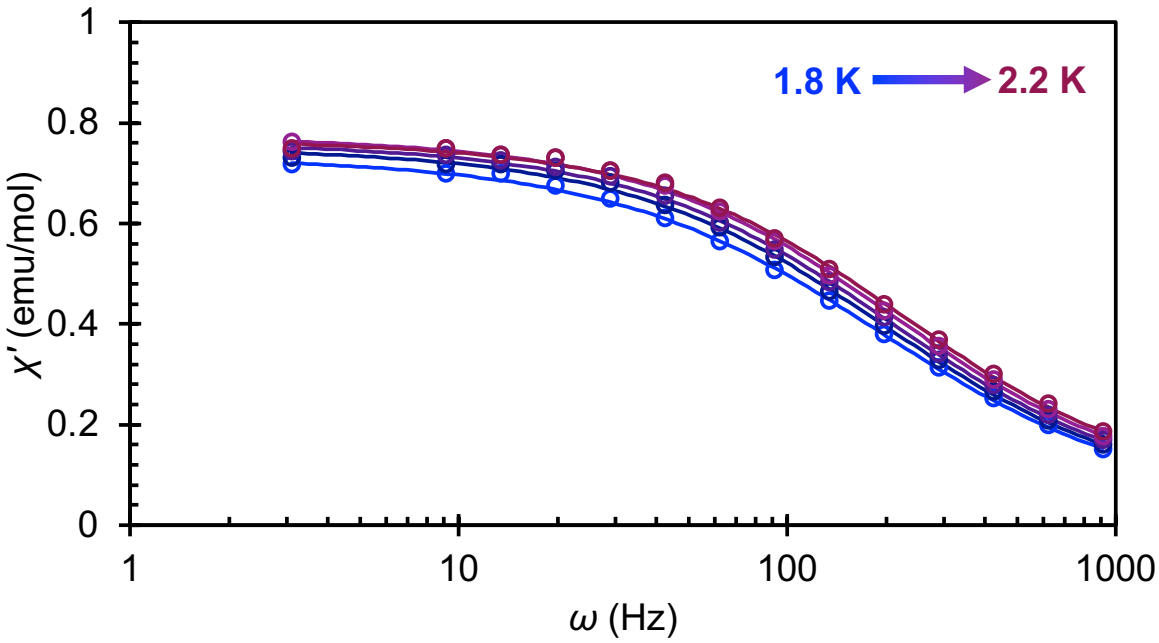

Figure S55 In-phase (χ') AC susceptibility for **4**, fitted with generalised Debye model in the temperature range 1.8-2.2 K under 0.2 T DC field.

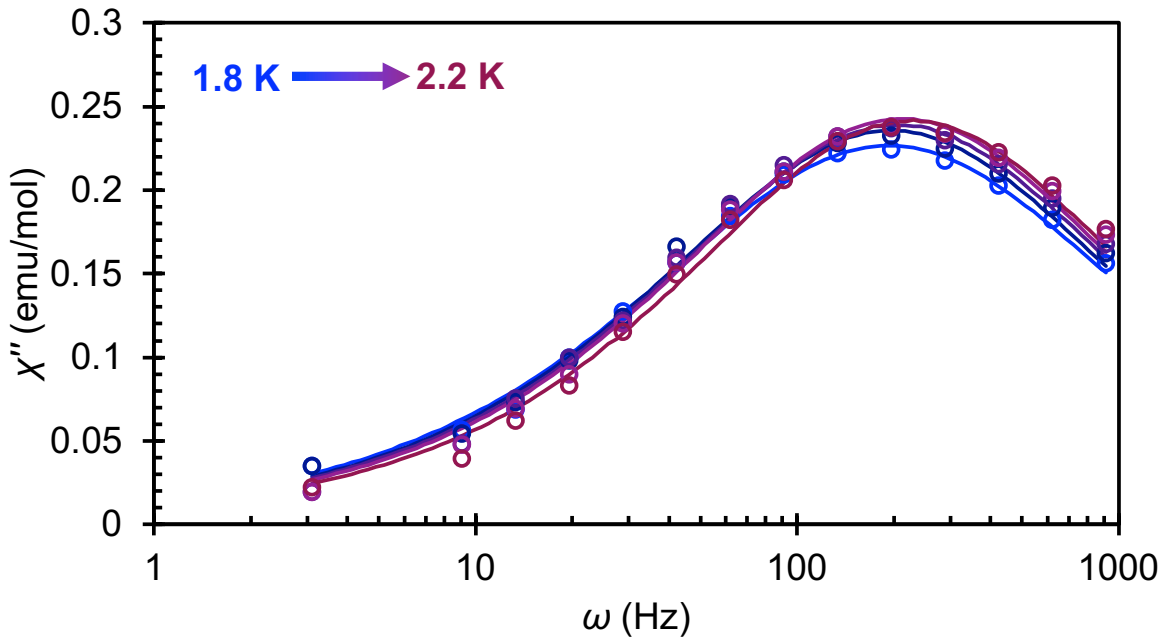

Figure S56 Out-of-phase (χ'') AC susceptibility for **4**, fitted with generalised Debye model in the temperature range 1.8-2.2 K under 0.2 T DC field.

Table S6 Table of extracted constant temperature susceptibility (χT), adiabatic susceptibility (χS), parameter gauging the width of distribution of relaxation times (α) and relaxation time (τ) at each individual temperature, for compound **4** under an applied field of 0.2 T

T (K)	χT (emu/mol)	χS (emu/mol)	α	τ (s)
1.80	0.74	0.03	0.27	0.00304(1)
1.90	0.75	0.04	0.25	0.00278(2)
2.00	0.76	0.05	0.25	0.00263(1)
2.10	0.78	0.05	0.25	0.00248(1)
2.20	0.77	0.06	0.24	0.00225(2)

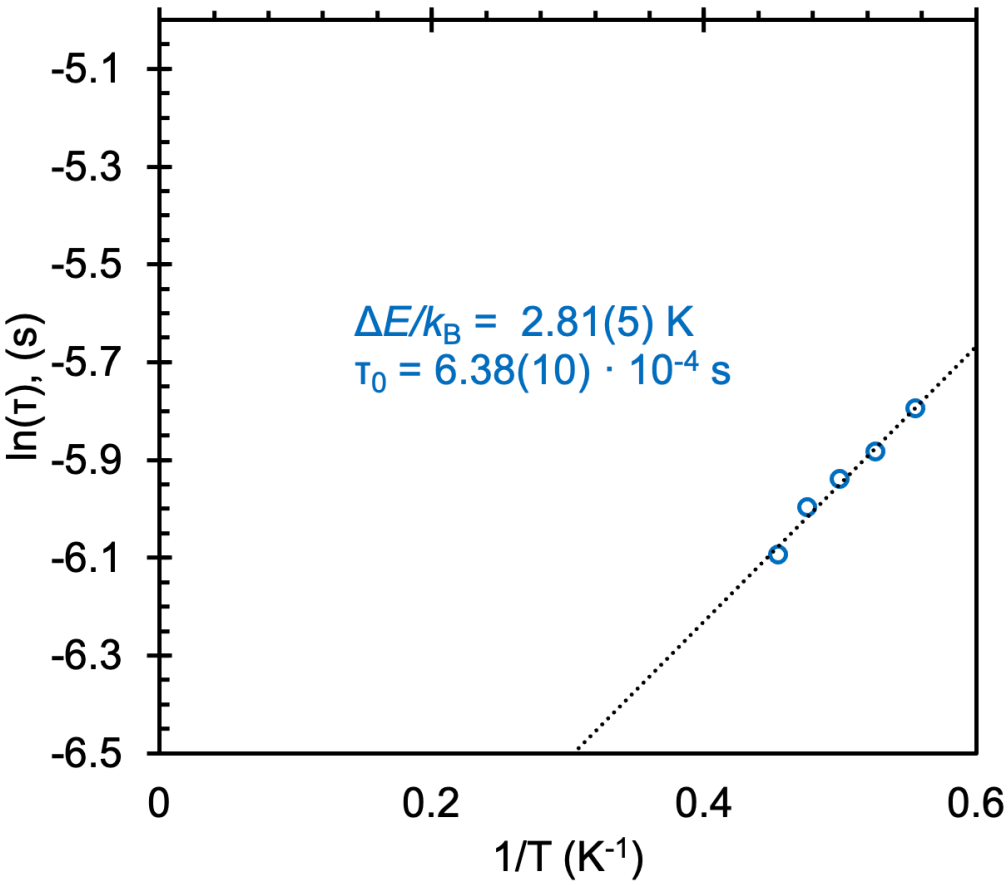

Figure S57 Arrhenius plot of **4** in the temperature region 1.8-2.2 K under 0.2 T DC field, with the obtained parameters of $\Delta E/k_B$ = 2.81(5) K, τ_0 = 6.38(10) · 10^{-4} s. The fit is extended to show linearity.

Computational data

All the DFT calculations were performed using Gaussian09 suite of programs.[12] Hybrid DFT functional (B3PW91) along with relativistic effective core potential and its associated basis sets for U, Si atoms with additional polarization functions for silicon atoms were employed.[13,14] Pople (6-31G**) basis set were used for the rest of the atoms.[15] NBO analysis were carried out with the NBO6.0. CASSCF calculations were also conducted on complexes **2** and **4** by distributing either 7 or 5 electrons into 7 and 5 orbitals, respectively. In both cases, the active molecular orbitals were obtained by a ROHF calculation on the highest spin state (octet and sextet).

Table S7 Different spin states computed with DFT for complexes **1**-**4**.

1: U_2bpym	**ΔH (kcal/mol)**
s = 2	0.0
s = 3	7.3
2: $[U_2bpym]^{1-}$	**ΔH (kcal/mol)**
s = 7/2	1.8
s = 5/2	0.0
3: $[U_2bpym]^{2-}$	**ΔH (kcal/mol)**
s = 3	0.0
s = 2	16.0
4: $[U_2bpym]^{1+}$	**ΔH (kcal/mol)**
s = 5/2	1.5
s = 3/2	0.0
s = 1/2	8.4

Table S8 Different spin states computed with CASSCF for complexes **1**-**4**.

2: $[U_2bpym]^{1-}$	**ΔH (kcal/mol)**
s = 7/2	2.3
s = 5/2	0.0
4: $[U_2bpym]^{1+}$	**ΔH (kcal/mol)**
s = 5/2	2.1
s = 3/2	0.0

Table S9 DFT computed bond distances (Å) for complexes **1**-**4**.

Bond	**1**	**2**	**3**	**4**
U1–N1	2.54	2.64	2.58	2.63
U1–N4	2.51	2.65	2.58	2.64
U2–N2	2.51	2.65	2.58	2.65
U2–N3	2.54	2.64	2.58	2.63
C1–C2	1.35	1.40	1.36	1.41

Table S10 DFT computed spin density values for complexes **1**-**4**.

Atom Labels	**1**	**2**	**3**	**4**
U1	2.18	3.02	3.11	2.16
U2	2.18	3.01	3.11	2.15
C1	0.00	-0.14	0.01	-0.18
C2	0.00	-0.14	0.01	-0.19

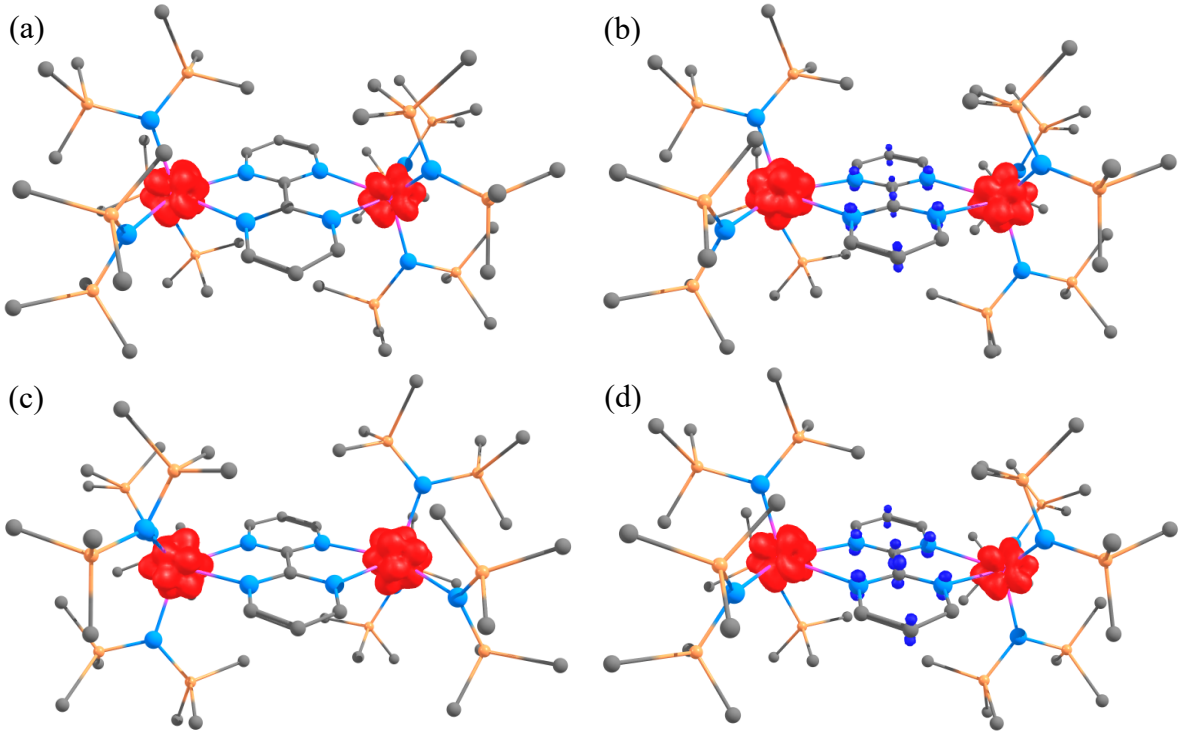

Figure S58 DFT computed spin density plots for complexes (a) **1**, (b) **2**, (c) **3** and (d) **4**.

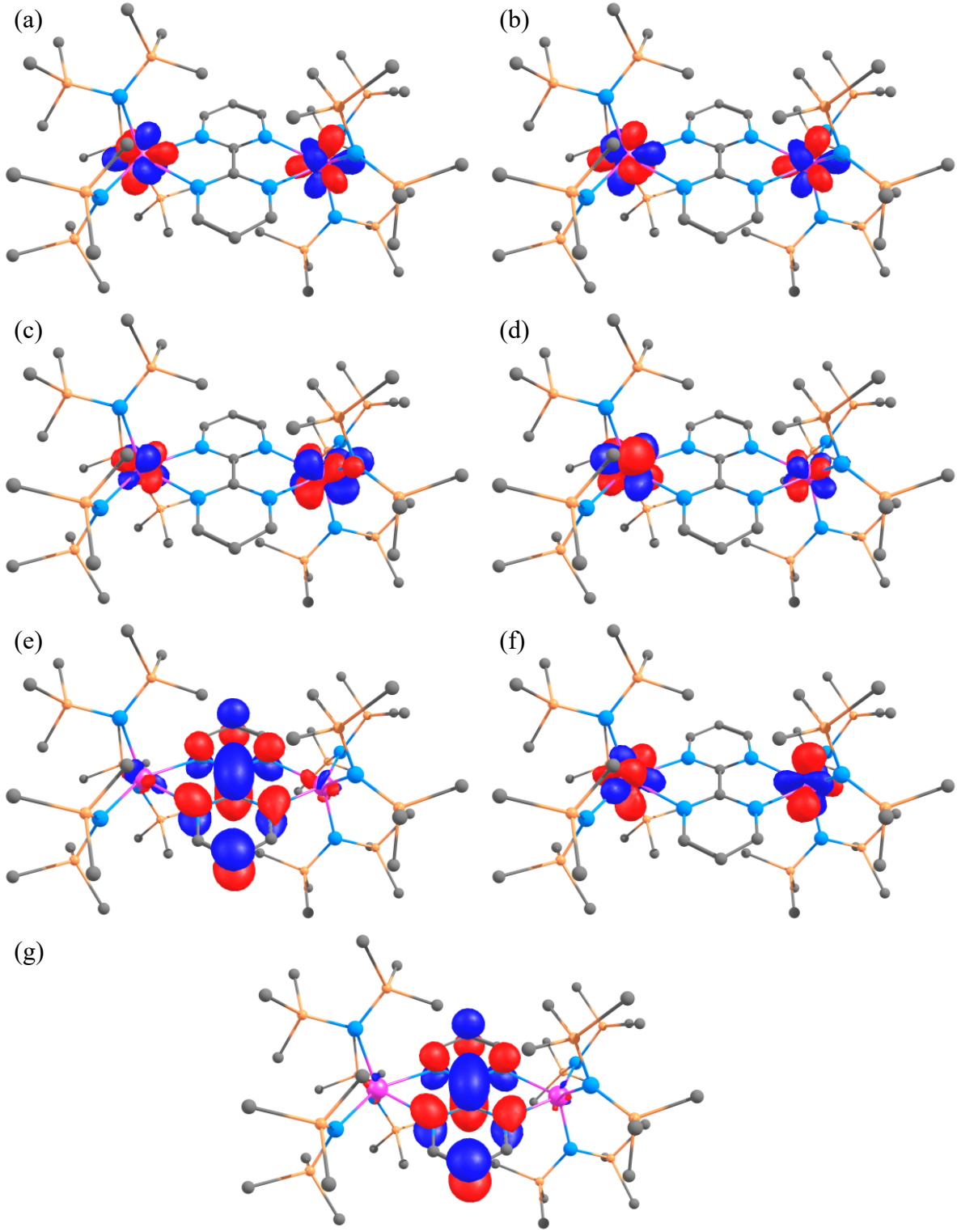

Figure S59 DFT computed MO's for complex **1** (a) Alpha Molecular orbital, AMO-HOMO-4 (b) AMO-HOMO-3 (c) AMO-HOMO-2 (d) AMO-HOMO-1 (e) AMO-HOMO (f) AMO-LUMO (g) Beta Molecular orbital, BMO-HOMO.

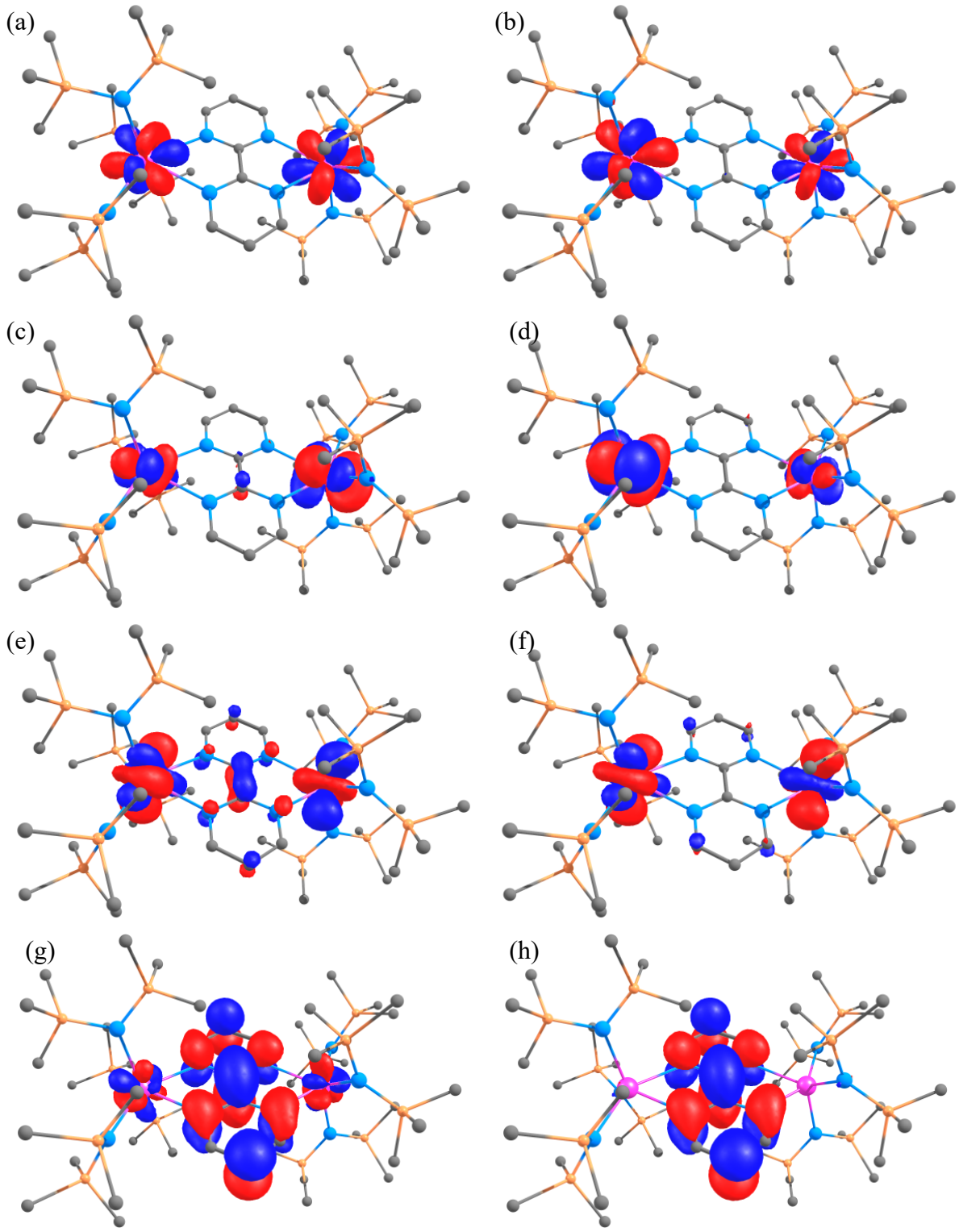

Figure S60 DFT computed MO's for complex **2** (a) Alpha Molecular orbital, AMO-HOMO-5 (b) AMO-HOMO-4 (c) AMO-HOMO-3 (d) AMO-HOMO-2 (e) AMO-HOMO-1 (f) AMO-HOMO (g) AMO-LUMO (h) Beta Molecular orbital, BMO-HOMO

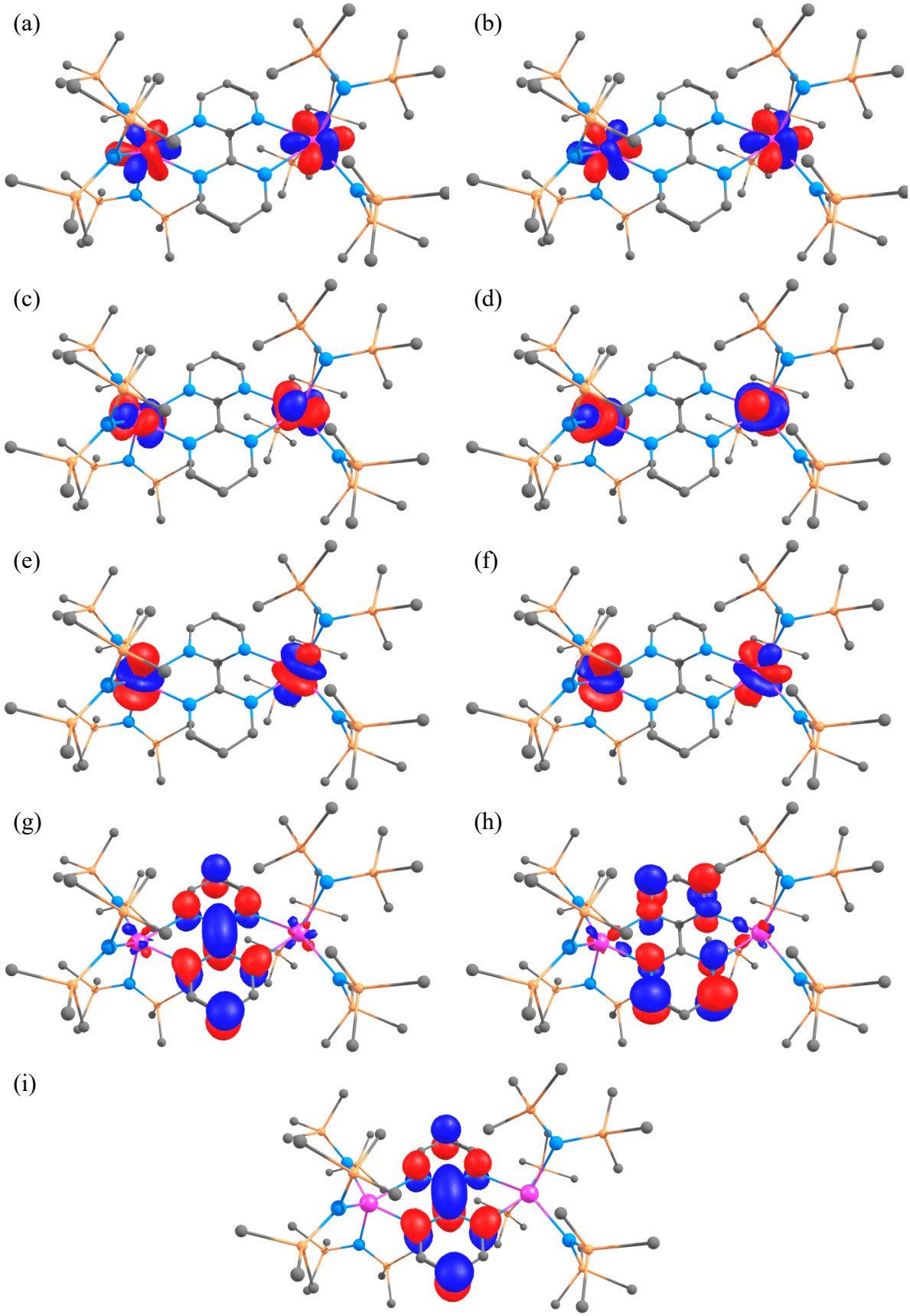

Figure S61 DFT computed MO's for complex **3** (a) Alpha Molecular orbital, AMO-HOMO-6 (b) AMO-HOMO-5 (c) AMO-HOMO-4 (d) AMO-HOMO-3 (e) AMO-HOMO-2 (f) AMO-HOMO-1 (g) AMO-HOMO (h) AMO-LUMO (i) Beta Molecular orbital, BMO-HOMO.

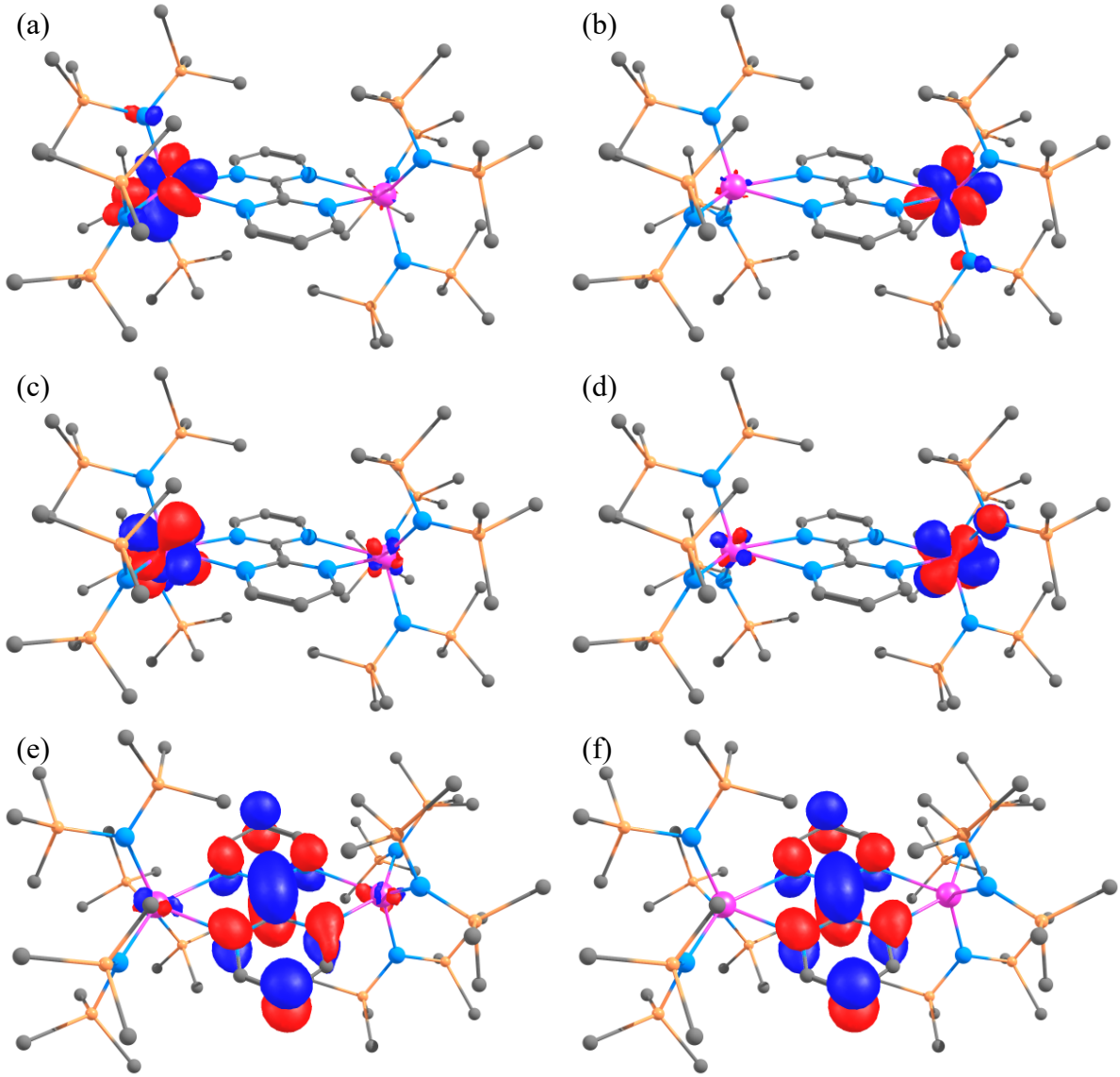

Figure S62 DFT computed MO's for complex **4** (a) Alpha Molecular orbital, AMO-HOMO-3 (b) AMO-HOMO-2 (c) AMO-HOMO-1 (d) AMO-HOMO (e) AMO-LUMO (f) Beta Molecular orbital, BMO-HOMO.

Optimized coordinates

Complex 1 (s=2)

U	7.721485000	0.555455000	9.437432000
Si	10.858676000	0.891052000	10.922088000
Si	9.451063000	3.520219000	10.794339000
Si	9.604403000	0.036189000	6.369034000
Si	6.749562000	-0.865020000	6.283557000
Si	5.560112000	3.019472000	8.039330000
Si	4.347946000	1.459821000	10.304723000
N	7.392560000	-0.035292000	11.887009000
N	6.957631000	-1.810488000	13.565027000
N	9.403742000	1.782342000	10.372938000
N	8.055799000	-0.112925000	7.261193000
N	5.788120000	1.740784000	9.273273000
C	7.253303000	-1.388542000	12.243922000
C	6.729350000	-0.835511000	14.444031000
H	6.442730000	-1.166275000	15.437130000
C	6.852462000	0.521311000	14.153434000
H	6.687673000	1.278372000	14.908391000
C	7.220274000	0.858404000	12.839338000
H	7.369753000	1.897810000	12.556316000
C	10.987459000	-0.752764000	9.989202000
H	10.077092000	-1.359510000	10.001946000
H	11.765750000	-1.354381000	10.471528000
H	11.294372000	-0.587404000	8.954537000
C	12.496664000	1.775804000	10.521973000
H	12.591659000	1.976901000	9.450719000
H	13.319050000	1.108423000	10.806682000
H	12.639001000	2.716368000	11.059487000
C	10.843531000	0.486515000	12.773585000
H	10.836764000	1.378641000	13.403283000
H	11.740800000	-0.091609000	13.022510000
H	9.971553000	-0.120244000	13.029958000
C	10.382772000	4.534968000	9.486386000
H	11.436279000	4.245291000	9.438176000
H	10.339635000	5.599171000	9.746050000
H	9.963430000	4.417086000	8.483644000
C	10.278003000	3.915263000	12.465837000
H	9.746807000	3.445265000	13.299645000
H	10.208572000	5.000962000	12.608217000
H	11.333498000	3.644371000	12.537316000
C	7.702566000	4.231069000	11.009254000
H	7.677316000	5.265320000	10.649096000
H	7.431302000	4.251257000	12.070510000
H	6.931915000	3.664903000	10.483100000
C	10.630640000	1.488085000	7.033825000
H	10.289704000	2.415033000	6.560694000
H	11.683075000	1.346797000	6.762089000
H	10.570844000	1.634706000	8.114101000
C	10.605995000	-1.581762000	6.430317000
H	10.709249000	-1.995257000	7.436114000
H	11.613307000	-1.410356000	6.033142000
H	10.134072000	-2.345104000	5.804018000
C	9.439456000	0.431662000	4.514656000
H	9.012718000	-0.382369000	3.923040000
H	10.454196000	0.609466000	4.137297000
H	8.856711000	1.337806000	4.327379000
C	6.169625000	0.223212000	4.831732000
H	6.276699000	1.291483000	5.028791000
H	5.111815000	0.026584000	4.624455000
H	6.728446000	-0.008033000	3.921461000
C	7.226209000	-2.522198000	5.466787000
H	8.038418000	-2.422843000	4.741184000
H	6.344576000	-2.873531000	4.916336000
H	7.496008000	-3.309439000	6.175763000
C	5.240699000	-1.252489000	7.365843000
H	5.436000000	-2.051724000	8.086342000
H	4.430258000	-1.592876000	6.710583000
H	4.883005000	-0.372742000	7.906529000
C	4.886729000	4.666402000	8.715687000
H	3.876518000	4.564691000	9.123874000
H	4.824399000	5.368114000	7.874707000
H	5.519813000	5.118805000	9.481276000
C	7.240541000	3.389397000	7.242592000
H	7.963161000	3.778934000	7.965271000
H	7.110146000	4.156199000	6.470434000
H	7.664622000	2.501920000	6.763682000
C	4.342853000	2.554249000	6.651249000
H	4.635824000	3.064080000	5.726373000
H	3.328004000	2.878572000	6.895160000
H	4.311988000	1.483492000	6.444468000
C	4.240354000	2.683160000	11.752576000
H	5.071480000	2.569049000	12.452905000
H	3.314628000	2.496786000	12.309884000
H	4.222633000	3.722109000	11.411953000
C	4.331920000	-0.299716000	11.015179000
H	4.937324000	-1.015352000	10.452159000
H	3.301860000	-0.671192000	10.997233000
H	4.674425000	-0.314171000	12.051767000
C	2.699016000	1.624067000	9.366050000
H	2.487779000	2.636935000	9.013893000
H	1.901065000	1.351522000	10.067647000
H	2.634054000	0.943694000	8.512046000
N	7.262721000	-3.673924000	11.632464000
N	7.697362000	-1.898608000	9.954553000
C	7.401627000	-2.320649000	11.275603000
C	7.926661000	-2.873499000	9.075688000
H	8.213661000	-2.542531000	8.082757000
C	7.804175000	-4.230348000	9.366302000
H	7.969763000	-4.987371000	8.611481000
C	7.435866000	-4.567562000	10.680253000
H	7.286688000	-5.607022000	10.963219000
U	6.932607000	-4.264655000	14.081973000
Si	3.796358000	-4.600212000	12.595719000
Si	5.204310000	-7.229262000	12.723107000
Si	5.047554000	-3.746819000	17.149413000
Si	7.902175000	-2.845732000	17.237412000
Si	9.093567000	-6.728912000	15.480659000
Si	10.306618000	-5.167958000	13.216562000
N	5.251116000	-5.491547000	13.145260000
N	6.596750000	-3.597275000	16.258291000
N	8.865950000	-5.449778000	14.247103000
C	3.667368000	-2.956624000	13.528950000
H	4.577539000	-2.349576000	13.515907000
H	2.888746000	-2.355186000	13.046938000
H	3.360829000	-3.122142000	14.563693000
C	2.158266000	-5.485173000	12.994940000
H	2.063047000	-5.687114000	14.066010000
H	1.335954000	-4.817542000	12.710601000
H	2.015978000	-6.425314000	12.456661000
C	3.812183000	-4.195001000	10.744385000

H	3.818466000	-5.086794000	10.114217000
H	2.915375000	-3.616103000	10.495594000
H	4.684636000	-3.588706000	10.488530000
C	4.272192000	-8.244660000	14.030258000
H	3.218740000	-7.954777000	14.078452000
H	4.315138000	-9.308703000	13.769903000
H	4.691366000	-8.127530000	15.033155000
C	4.378086000	-7.623678000	11.051121000
H	4.909633000	-7.153341000	10.217728000
H	4.447553000	-8.709319000	10.908327000
H	3.322629000	-7.352733000	10.979333000
C	6.953020000	-7.939749000	12.508667000
H	6.978201000	-8.974236000	12.868151000
H	7.224922000	-7.959188000	11.447560000
H	7.723292000	-7.373832000	13.035656000
C	4.021782000	-5.198447000	16.483339000
H	4.362348000	-6.125539000	16.956456000
H	2.969127000	-5.057256000	16.754269000
H	4.082472000	-5.344729000	15.403073000
C	4.046314000	-2.128658000	17.088275000
H	3.944183000	-1.714384000	16.082686000
H	3.038583000	-2.300016000	17.484402000
H	4.517944000	-1.365952000	17.715572000
C	5.211120000	-4.143237000	19.003726000
H	5.637302000	-3.329505000	19.596150000
H	4.196053000	-4.321259000	19.380110000
H	5.793708000	-5.049471000	19.191054000
C	8.481331000	-3.934929000	18.688814000
H	8.374688000	-5.003076000	18.490850000
H	9.538931000	-3.738194000	18.897045000
H	7.921745000	-3.704521000	19.598827000
C	7.424470000	-1.189357000	18.055221000
H	6.613633000	-1.290229000	18.782145000
H	8.306468000	-0.836761000	18.604272000
H	7.152116000	-0.402374000	17.346954000
C	9.411710000	-2.457132000	16.156432000
H	9.216850000	-1.657232000	15.436552000
H	10.221711000	-2.117347000	16.812549000
H	9.769797000	-3.336349000	15.615133000
C	9.767532000	-8.375438000	14.803910000
H	10.778033000	-8.273409000	14.396513000
H	9.829312000	-9.077601000	15.644554000
H	9.135040000	-8.827485000	14.037620000
C	7.412804000	-7.099353000	16.276428000
H	6.690715000	-7.488968000	15.553263000
H	7.542885000	-7.866211000	17.048581000
H	6.988217000	-6.212016000	16.755153000
C	10.310158000	-6.264059000	16.869455000
H	10.016947000	-6.774411000	17.793967000
H	11.325179000	-6.588032000	16.625792000
H	10.340713000	-5.193398000	17.076777000
C	10.415504000	-6.390604000	11.768224000
H	9.585058000	-6.276119000	11.067152000
H	11.341762000	-6.203932000	11.211900000
H	10.432915000	-7.429725000	12.108339000
C	10.322444000	-3.408015000	12.507024000
H	9.715427000	-2.693126000	13.069260000
H	11.352139000	-3.035638000	12.526933000
H	9.981702000	-3.393371000	11.469857000
C	11.955071000	-5.332121000	14.156068000
H	12.166377000	-6.345025000	14.508071000
H	12.753321000	-5.059184000	13.454963000
H	12.019378000	-4.651938000	15.010274000

Complex 1 (s=3)

U	7.725342000	0.570346000	9.426697000
Si	10.881764000	0.901184000	10.845121000
Si	9.515759000	3.553667000	10.708707000
Si	9.579824000	-0.000856000	6.324048000
Si	6.712684000	-0.844570000	6.279336000
Si	5.534560000	3.018039000	8.087838000
Si	4.347395000	1.491822000	10.381587000
N	7.457272000	-0.070528000	11.835368000
N	7.051732000	-1.787330000	13.513467000
N	9.433958000	1.810816000	10.322797000
N	8.045608000	-0.127343000	7.238691000
N	5.773338000	1.745599000	9.326528000
C	7.303396000	-1.371687000	12.230662000
C	6.855328000	-0.804488000	14.426768000
H	6.588027000	-1.135586000	15.422222000
C	7.004023000	0.543028000	14.105856000
H	6.875093000	1.309591000	14.860828000
C	7.340455000	0.874151000	12.800736000
H	7.511186000	1.899118000	12.492412000
C	10.926943000	-0.768705000	9.945348000
H	10.008348000	-1.360980000	9.997157000
H	11.705941000	-1.378889000	10.415220000
H	11.203461000	-0.635620000	8.897693000
C	12.529367000	1.723477000	10.364463000
H	12.596197000	1.895099000	9.286253000
H	13.343491000	1.043459000	10.642747000
H	12.710957000	2.673624000	10.872580000
C	10.943839000	0.544584000	12.706146000
H	11.035169000	1.454120000	13.303727000
H	11.815931000	-0.084081000	12.919278000
H	10.053954000	0.005327000	13.039728000
C	10.407992000	4.542802000	9.353906000
H	11.455362000	4.238077000	9.271315000
H	10.389503000	5.610000000	9.604207000
H	9.951850000	4.421931000	8.367584000
C	10.409321000	3.970925000	12.340194000
H	9.917874000	3.505652000	13.200537000
H	10.338450000	5.057562000	12.474272000
H	11.469390000	3.708890000	12.368511000
C	7.779468000	4.274670000	10.978454000
H	7.749595000	5.313763000	10.632918000
H	7.533510000	4.280895000	12.046142000
H	6.993567000	3.718712000	10.464373000
C	10.626998000	1.449028000	6.959786000
H	10.281842000	2.373850000	6.485155000
H	11.674414000	1.302353000	6.672100000
H	10.584758000	1.605161000	8.039537000
C	10.568269000	-1.628590000	6.378930000
H	10.672476000	-2.046754000	7.382968000
H	11.575286000	-1.467800000	5.976765000
H	10.085141000	-2.385630000	5.752992000
C	9.394173000	0.383325000	4.468588000
H	8.944400000	-0.426195000	3.887923000
H	10.405896000	0.541443000	4.074739000
H	8.824615000	1.298567000	4.284696000
C	6.117790000	0.259803000	4.846013000
H	6.225998000	1.325922000	5.054340000
H	5.058176000	0.064789000	4.646323000
H	6.668159000	0.039472000	3.927962000
C	7.138892000	-2.505553000	5.439906000
H	7.942833000	-2.414901000	4.704040000

H	6.242942000	-2.833793000	4.898470000
H	7.404065000	-3.307038000	6.134790000
C	5.222848000	-1.208506000	7.397593000
H	5.419594000	-2.017267000	8.107379000
H	4.385556000	-1.526743000	6.765774000
H	4.900405000	-0.324094000	7.953494000
C	4.883670000	4.674154000	8.762998000
H	3.877545000	4.583060000	9.183364000
H	4.817700000	5.372260000	7.919343000
H	5.529444000	5.124692000	9.518978000
C	7.209290000	3.369622000	7.269474000
H	7.943045000	3.753732000	7.983859000
H	7.076889000	4.138283000	6.499455000
H	7.622645000	2.480126000	6.784342000
C	4.296657000	2.554688000	6.718089000
H	4.570403000	3.073699000	5.792448000
H	3.284269000	2.870440000	6.982050000
H	4.269079000	1.485385000	6.503463000
C	4.293228000	2.719592000	11.827602000
H	5.155706000	2.605187000	12.489508000
H	3.392031000	2.537185000	12.424851000
H	4.263357000	3.757367000	11.484301000
C	4.300801000	-0.260649000	11.106483000
H	4.717069000	-1.019225000	10.437808000
H	3.252023000	-0.525507000	11.279356000
H	4.815322000	-0.321326000	12.066979000
C	2.683582000	1.668260000	9.471713000
H	2.480219000	2.678583000	9.108123000
H	1.894379000	1.417879000	10.191109000
H	2.592768000	0.976548000	8.629115000
N	7.275932000	-3.665284000	11.618294000
N	7.658941000	-1.939514000	9.945389000
C	7.412002000	-2.359638000	11.232423000
C	7.865999000	-2.914386000	9.038194000
H	8.122456000	-2.576535000	8.041411000
C	7.751148000	-4.262618000	9.352250000
H	7.900947000	-5.026956000	8.599595000
C	7.421318000	-4.595862000	10.667578000
H	7.277742000	-5.625323000	10.976603000
U	6.935070000	-4.264077000	14.103136000
Si	3.837717000	-4.638509000	12.566927000
Si	5.256912000	-7.263424000	12.698310000
Si	4.918888000	-3.793266000	17.143279000
Si	7.758144000	-2.897075000	17.328389000
Si	9.130023000	-6.685209000	15.491404000
Si	10.401896000	-5.087432000	13.300134000
N	5.281892000	-5.530327000	13.111841000
N	6.487763000	-3.626119000	16.305847000
N	8.934354000	-5.391449000	14.273506000
C	3.744614000	-2.986727000	13.494483000
H	4.664090000	-2.391965000	13.483301000
H	2.980144000	-2.368559000	13.011712000
H	3.435451000	-3.141189000	14.529604000
C	2.184608000	-5.497359000	12.960203000
H	2.080826000	-5.705021000	14.029037000
H	1.369893000	-4.821726000	12.673036000
H	2.038266000	-6.433861000	12.415821000
C	3.827541000	-4.233224000	10.711577000
H	3.800781000	-5.127746000	10.085284000
H	2.936868000	-3.637573000	10.480420000
H	4.704243000	-3.645423000	10.427713000
C	4.332958000	-8.298877000	13.996472000
H	3.279412000	-8.009456000	14.051894000
H	4.374810000	-9.359591000	13.722410000
H	4.755315000	-8.195319000	14.999695000
C	4.435740000	-7.669656000	11.025286000
H	4.953049000	-7.185299000	10.190807000
H	4.521502000	-8.753114000	10.875729000
H	3.375024000	-7.415600000	10.961771000
C	7.020316000	-7.943962000	12.492601000
H	7.070126000	-8.973083000	12.864443000
H	7.296269000	-7.969809000	11.432348000
H	7.776613000	-7.354222000	13.015047000
C	3.930453000	-5.251523000	16.435838000
H	4.272133000	-6.178107000	16.909603000
H	2.867136000	-5.132410000	16.673561000
H	4.031751000	-5.384580000	15.357005000
C	3.904124000	-2.181251000	17.068107000
H	3.892108000	-1.719605000	16.077855000
H	2.865823000	-2.371399000	17.363848000
H	4.314146000	-1.447498000	17.769400000
C	5.017495000	-4.207153000	19.000608000
H	5.422149000	-3.400310000	19.617399000
H	3.991100000	-4.391782000	19.341501000
H	5.595816000	-5.114698000	19.196003000
C	8.319735000	-4.000538000	18.775861000
H	8.282210000	-5.064961000	18.535247000
H	9.353350000	-3.756391000	19.046230000
H	7.701809000	-3.834986000	19.661846000
C	7.249982000	-1.252296000	18.155413000
H	6.451515000	-1.383062000	18.891422000
H	8.124959000	-0.867122000	18.693359000
H	6.934084000	-0.475360000	17.453315000
C	9.295552000	-2.489808000	16.289963000
H	9.107212000	-1.700237000	15.556276000
H	10.082190000	-2.129297000	16.963019000
H	9.680281000	-3.369021000	15.766491000
C	9.821394000	-8.325939000	14.813543000
H	10.838525000	-8.221658000	14.423606000
H	9.868324000	-9.036647000	15.647970000
H	9.202260000	-8.770762000	14.032187000
C	7.423512000	-7.068992000	16.226444000
H	6.721540000	-7.432035000	15.469816000
H	7.525745000	-7.861706000	16.976453000
H	6.985879000	-6.196294000	16.721023000
C	10.297733000	-6.247662000	16.931376000
H	9.989758000	-6.800091000	17.826666000
H	11.326748000	-6.539595000	16.706320000
H	10.297561000	-5.185400000	17.181638000
C	10.506477000	-6.225045000	11.783230000
H	9.713084000	-6.020555000	11.059455000
H	11.465411000	-6.075140000	11.273663000
H	10.439513000	-7.278556000	12.069081000
C	10.515529000	-3.292099000	12.707618000
H	10.467173000	-2.587747000	13.542448000
H	11.490179000	-3.161481000	12.223671000
H	9.751085000	-3.018678000	11.979568000
C	12.032439000	-5.334517000	14.255100000
H	12.213939000	-6.366474000	14.565774000
H	12.850877000	-5.049040000	13.583097000
H	12.094721000	-4.695397000	15.140615000

Complex 2 (s=5/2)

U	7.708237000	0.659038000	9.367552000
Si	10.870423000	1.017594000	10.914209000

Si	9.485730000	3.654705000	10.736503000
Si	9.677728000	0.076430000	6.277143000
Si	6.825897000	-0.758328000	6.090882000
Si	5.480158000	3.127168000	7.955630000
Si	4.257632000	1.535664000	10.184053000
N	7.431740000	-0.050099000	11.892648000
N	7.032724000	-1.791562000	13.554453000
N	9.456886000	1.930436000	10.378630000
N	8.113759000	-0.064969000	7.081022000
N	5.663788000	1.855945000	9.164041000
C	7.277069000	-1.371122000	12.260232000
C	6.880471000	-0.838761000	14.469776000
H	6.637628000	-1.189909000	15.468437000
C	7.026675000	0.520947000	14.181959000
H	6.921668000	1.277131000	14.949541000
C	7.327968000	0.854538000	12.859127000
H	7.489846000	1.886621000	12.559111000
C	10.887524000	-0.700181000	10.107621000
H	10.001179000	-1.300084000	10.334581000
H	11.750437000	-1.255919000	10.492219000
H	10.999367000	-0.632797000	9.022876000
C	12.540740000	1.800353000	10.416395000
H	12.615890000	1.928483000	9.332345000
H	13.355899000	1.138139000	10.732733000
H	12.710707000	2.774971000	10.883209000
C	10.963885000	0.713144000	12.790680000
H	11.050034000	1.638949000	13.365082000
H	11.844275000	0.098792000	13.013621000
H	10.084141000	0.171333000	13.148364000
C	10.346646000	4.672913000	9.373932000
H	11.402061000	4.393682000	9.293011000
H	10.298134000	5.743475000	9.607168000
H	9.893418000	4.520630000	8.390278000
C	10.374770000	4.150401000	12.356956000
H	9.903202000	3.689150000	13.231004000
H	10.283530000	5.237968000	12.471469000
H	11.440753000	3.907029000	12.379592000
C	7.729082000	4.339473000	10.991704000
H	7.690980000	5.403827000	10.732264000
H	7.434964000	4.251530000	12.044124000
H	6.977473000	3.811439000	10.400067000
C	10.691240000	1.520758000	6.985280000
H	10.348858000	2.456882000	6.530041000
H	11.752116000	1.399036000	6.736136000
H	10.601830000	1.640509000	8.068002000
C	10.695728000	-1.537722000	6.371208000
H	10.769823000	-1.939259000	7.385401000
H	11.714087000	-1.375864000	5.998071000
H	10.233841000	-2.309417000	5.746047000
C	9.626708000	0.478418000	4.407739000
H	9.205349000	-0.324221000	3.795339000
H	10.658817000	0.639346000	4.071581000
H	9.065294000	1.395406000	4.203798000
C	6.265800000	0.352769000	4.641374000
H	6.246862000	1.410081000	4.916232000
H	5.254107000	0.071670000	4.325287000
H	6.924315000	0.243552000	3.775487000
C	7.275818000	-2.421658000	5.251231000
H	8.091176000	-2.318871000	4.528149000
H	6.397414000	-2.783338000	4.702245000
H	7.558211000	-3.204702000	5.962258000
C	5.274163000	-1.129000000	7.123771000
H	5.444268000	-1.920460000	7.860066000
H	4.470219000	-1.464895000	6.457661000
H	4.927875000	-0.237914000	7.655150000
C	4.859857000	4.805391000	8.626363000
H	3.855202000	4.730124000	9.054691000
H	4.806451000	5.519580000	7.795092000
H	5.520335000	5.226326000	9.388230000
C	7.172039000	3.462127000	7.157605000
H	7.881691000	3.875056000	7.881231000
H	7.065725000	4.197694000	6.351656000
H	7.602851000	2.552083000	6.725841000
C	4.256074000	2.718363000	6.548450000
H	4.489054000	3.328245000	5.667209000
H	3.227094000	2.944519000	6.841895000
H	4.296140000	1.669128000	6.247880000
C	4.245489000	2.603667000	11.760160000
H	5.081386000	2.363956000	12.423121000
H	3.319303000	2.443653000	12.324985000
H	4.310583000	3.667471000	11.510390000
C	4.157129000	-0.289366000	10.692617000
H	3.881597000	-0.914678000	9.838214000
H	3.379586000	-0.405777000	11.456010000
H	5.083451000	-0.686174000	11.114167000
C	2.565108000	1.854208000	9.355515000
H	2.387727000	2.905341000	9.109506000
H	1.782877000	1.546459000	10.060493000
H	2.439191000	1.263396000	8.443184000
N	7.207531000	-3.662456000	11.624395000
N	7.608902000	-1.921349000	9.962258000
C	7.363456000	-2.341386000	11.256492000
C	7.753459000	-2.874239000	9.045809000
H	7.995403000	-2.523939000	8.046663000
C	7.601703000	-4.233577000	9.333071000
H	7.700841000	-4.989641000	8.564601000
C	7.305594000	-4.567021000	10.657125000
H	7.143122000	-5.598863000	10.957661000
U	6.940307000	-4.367798000	14.149807000
Si	3.781119000	-4.747427000	12.612081000
Si	5.173146000	-7.381755000	12.799324000
Si	4.979680000	-3.791362000	17.247990000
Si	7.826257000	-2.934722000	17.420502000
Si	9.183649000	-6.818742000	15.556741000
Si	10.393864000	-5.229779000	13.320216000
N	5.198087000	-5.655276000	13.146277000
N	6.538158000	-3.635889000	16.435742000
N	8.991978000	-5.551230000	14.345924000
C	3.790735000	-3.012654000	13.381745000
H	4.626804000	-2.394920000	13.042538000
H	2.871749000	-2.494558000	13.084084000
H	3.801944000	-3.051912000	14.473878000
C	2.116453000	-5.517290000	13.147616000
H	2.049615000	-5.615102000	14.235246000
H	1.296290000	-4.867777000	12.818164000
H	1.946645000	-6.505865000	12.710677000
C	3.655888000	-4.476849000	10.731915000
H	3.510106000	-5.409051000	10.180435000
H	2.799649000	-3.825825000	10.518910000
H	4.549878000	-3.985186000	10.338806000
C	4.336641000	-8.399358000	14.177796000
H	3.283101000	-8.118983000	14.277431000
H	4.379506000	-9.469468000	13.941259000
H	4.806692000	-8.250781000	15.154081000
C	4.262253000	-7.891883000	11.195781000
H	4.715089000	-7.430331000	10.312145000

H	4.360645000	-8.979172000	11.084679000
H	3.193948000	-7.657516000	11.190642000
C	6.930643000	-8.055647000	12.522308000
H	7.684954000	-7.523428000	13.106859000
H	6.979480000	-9.120370000	12.778476000
H	7.211984000	-7.963008000	11.466789000
C	3.978015000	-5.245967000	16.544817000
H	4.325931000	-6.178157000	17.003781000
H	2.915679000	-5.130828000	16.790642000
H	4.070938000	-5.368588000	15.462571000
C	3.936605000	-2.192465000	17.161068000
H	3.792773000	-1.821468000	16.142664000
H	2.945401000	-2.361070000	17.599145000
H	4.419996000	-1.395091000	17.735597000
C	5.044286000	-4.188318000	19.117947000
H	5.458524000	-3.379310000	19.726847000
H	4.015422000	-4.360371000	19.458481000
H	5.617029000	-5.098194000	19.321940000
C	8.397415000	-4.039985000	18.870596000
H	8.414920000	-5.098552000	18.600387000
H	9.411462000	-3.757085000	19.177388000
H	7.745989000	-3.927301000	19.741388000
C	7.370953000	-1.271897000	18.258174000
H	6.554063000	-1.375577000	18.979434000
H	8.247385000	-0.908013000	18.808846000
H	7.089041000	-0.490002000	17.545667000
C	9.373822000	-2.559210000	16.383176000
H	9.199991000	-1.768432000	15.647080000
H	10.177925000	-2.220558000	17.047710000
H	9.722266000	-3.449316000	15.851547000
C	9.806523000	-8.496988000	14.888641000
H	10.810207000	-8.420526000	14.458277000
H	9.863026000	-9.209165000	15.721431000
H	9.145595000	-8.921131000	14.128962000
C	7.494219000	-7.155632000	16.358582000
H	6.781059000	-7.559340000	15.633173000
H	7.600519000	-7.899218000	17.157106000
H	7.067337000	-6.248307000	16.799686000
C	10.409351000	-6.402125000	16.959994000
H	10.179411000	-7.009047000	17.844057000
H	11.438335000	-6.626839000	16.665496000
H	10.367090000	-5.351739000	17.256283000
C	10.401287000	-6.299835000	11.745553000
H	9.561919000	-6.062320000	11.086148000
H	11.324555000	-6.138558000	11.176323000
H	10.339435000	-7.363541000	11.996566000
C	10.491686000	-3.405919000	12.808377000
H	10.758942000	-2.777420000	13.663026000
H	11.275538000	-3.290265000	12.051350000
H	9.568304000	-3.012403000	12.377546000
C	12.089388000	-5.545301000	14.143860000
H	12.268280000	-6.595546000	14.392473000
H	12.869007000	-5.239275000	13.435262000
H	12.218233000	-4.951604000	15.053916000

Complex 2 (s=7/2)

U	7.674462000	0.689372000	9.339883000
Si	10.846564000	1.005817000	10.925738000
Si	9.472097000	3.645923000	10.738535000
Si	9.645393000	0.058750000	6.269575000
Si	6.784016000	-0.750562000	6.071128000
Si	5.456251000	3.161460000	7.931339000
Si	4.214977000	1.583010000	10.159836000
N	7.363946000	-0.048671000	11.903779000
N	7.072589000	-1.798992000	13.561864000
N	9.439737000	1.921864000	10.382538000
N	8.075343000	-0.067574000	7.060924000
N	5.623533000	1.895270000	9.145058000
C	7.273089000	-1.368949000	12.269280000
C	6.911126000	-0.854005000	14.486585000
H	6.704686000	-1.218838000	15.488500000
C	6.996340000	0.508567000	14.200285000
H	6.879374000	1.259193000	14.971560000
C	7.247784000	0.853531000	12.868722000
H	7.360514000	1.890199000	12.562925000
C	10.876827000	-0.715015000	10.125165000
H	9.989919000	-1.315231000	10.347162000
H	11.738717000	-1.266012000	10.519033000
H	10.994820000	-0.651974000	9.040858000
C	12.521748000	1.787184000	10.442231000
H	12.604048000	1.913732000	9.358385000
H	13.334498000	1.125061000	10.764787000
H	12.688674000	2.762543000	10.908496000
C	10.919174000	0.699005000	12.803457000
H	10.986660000	1.624095000	13.381498000
H	11.801833000	0.092596000	13.038688000
H	10.039592000	0.147362000	13.146973000
C	10.346978000	4.658101000	9.380271000
H	11.403069000	4.378390000	9.310496000
H	10.296269000	5.730090000	9.606300000
H	9.902743000	4.499292000	8.393522000
C	10.348654000	4.142841000	12.365622000
H	9.867044000	3.686755000	13.236906000
H	10.262179000	5.231202000	12.476098000
H	11.413098000	3.893949000	12.398715000
C	7.717047000	4.341906000	10.976807000
H	7.694065000	5.410231000	10.731945000
H	7.406886000	4.243299000	12.023750000
H	6.967371000	3.831346000	10.367496000
C	10.665649000	1.494434000	6.985817000
H	10.327619000	2.435373000	6.537275000
H	11.725812000	1.369295000	6.735187000
H	10.578673000	1.607238000	8.069691000
C	10.649548000	-1.563033000	6.377084000
H	10.717059000	-1.955774000	7.395295000
H	11.670546000	-1.413241000	6.006223000
H	10.183152000	-2.336269000	5.757130000
C	9.610539000	0.458681000	4.399279000
H	9.183322000	-0.340589000	3.786423000
H	10.645527000	0.608676000	4.067039000
H	9.058799000	1.380775000	4.191612000
C	6.234985000	0.362930000	4.620009000
H	6.212734000	1.419144000	4.898777000
H	5.226774000	0.082015000	4.292830000
H	6.902562000	0.257423000	3.760574000
C	7.221267000	-2.419516000	5.235002000
H	8.041455000	-2.325370000	4.516111000
H	6.342528000	-2.774102000	4.681942000
H	7.492663000	-3.204528000	5.948389000
C	5.230300000	-1.108496000	7.106381000
H	5.392127000	-1.908578000	7.835501000
H	4.418967000	-1.428441000	6.441402000
H	4.897676000	-0.216981000	7.646147000
C	4.850482000	4.848548000	8.593390000
H	3.842909000	4.783585000	9.016670000
H	4.808529000	5.562377000	7.761197000

H	5.511212000	5.263542000	9.358488000
C	7.155077000	3.476190000	7.137673000
H	7.864077000	3.895923000	7.858186000
H	7.056852000	4.200623000	6.320633000
H	7.582991000	2.558500000	6.718623000
C	4.234801000	2.760303000	6.519697000
H	4.467865000	3.376310000	5.642687000
H	3.204871000	2.982517000	6.812901000
H	4.277304000	1.713050000	6.212493000
C	4.191455000	2.662341000	11.729271000
H	5.028183000	2.436532000	12.396028000
H	3.265634000	2.499606000	12.293909000
H	4.248588000	3.724589000	11.471136000
C	4.113162000	-0.238583000	10.684701000
H	3.845713000	-0.872065000	9.833750000
H	3.330103000	-0.350247000	11.443232000
H	5.037477000	-0.628271000	11.116473000
C	2.525305000	1.894525000	9.322690000
H	2.349722000	2.944417000	9.069626000
H	1.738676000	1.590843000	10.024515000
H	2.404918000	1.299111000	8.412543000
N	7.289489000	-3.660509000	11.616005000
N	7.581291000	-1.910226000	9.957974000
C	7.380587000	-2.340238000	11.250538000
C	7.742652000	-2.855229000	9.033258000
H	7.949361000	-2.490421000	8.031392000
C	7.657064000	-4.217790000	9.319506000
H	7.773929000	-4.968422000	8.548221000
C	7.405475000	-4.562723000	10.651052000
H	7.292521000	-5.599365000	10.956850000
U	6.979272000	-4.398807000	14.179635000
Si	3.806579000	-4.714559000	12.594973000
Si	5.180519000	-7.355051000	12.781517000
Si	5.009919000	-3.768050000	17.250853000
Si	7.871523000	-2.959031000	17.447921000
Si	9.197494000	-6.871334000	15.586642000
Si	10.438529000	-5.292982000	13.357994000
N	5.213385000	-5.631000000	13.137494000
N	6.579602000	-3.641832000	16.458789000
N	9.030154000	-5.604987000	14.373112000
C	3.777505000	-2.993474000	13.395062000
H	4.664156000	-2.393342000	13.171874000
H	2.915131000	-2.442606000	13.002075000
H	3.660778000	-3.056206000	14.479530000
C	2.131402000	-5.495124000	13.079817000
H	2.049607000	-5.621166000	14.163758000
H	1.318662000	-4.832944000	12.757355000
H	1.963974000	-6.470654000	12.614081000
C	3.732586000	-4.408598000	10.717167000
H	3.660750000	-5.333910000	10.140000000
H	2.851831000	-3.799102000	10.482790000
H	4.613705000	-3.860554000	10.371840000
C	4.306654000	-8.367268000	14.140422000
H	3.250802000	-8.086980000	14.211501000
H	4.356477000	-9.439165000	13.913739000
H	4.752063000	-8.209309000	15.126776000
C	4.302447000	-7.851925000	11.155237000
H	4.782894000	-7.395408000	10.283544000
H	4.389255000	-8.940223000	11.044406000
H	3.237855000	-7.603488000	11.123412000
C	6.935302000	-8.051196000	12.541644000
H	7.685598000	-7.540804000	13.150342000
H	6.958384000	-9.119560000	12.786339000
H	7.244533000	-7.952526000	11.494430000
C	3.989166000	-5.203483000	16.534811000
H	4.326964000	-6.144527000	16.983305000
H	2.929056000	-5.078044000	16.785510000
H	4.076013000	-5.316318000	15.450920000
C	4.005753000	-2.146218000	17.144018000
H	3.937336000	-1.753588000	16.125822000
H	2.985077000	-2.296024000	17.515764000
H	4.472635000	-1.372889000	17.763488000
C	5.045670000	-4.168188000	19.121077000
H	5.473334000	-3.369046000	19.733792000
H	4.010845000	-4.318087000	19.453864000
H	5.597403000	-5.090379000	19.328330000
C	8.421308000	-4.072574000	18.898709000
H	8.443702000	-5.128757000	18.619841000
H	9.429582000	-3.791454000	19.225523000
H	7.754046000	-3.967291000	19.758414000
C	7.434749000	-1.290025000	18.284177000
H	6.615014000	-1.384127000	19.003592000
H	8.313786000	-0.935171000	18.836584000
H	7.162776000	-0.505262000	17.570737000
C	9.424707000	-2.601333000	16.411812000
H	9.262487000	-1.801650000	15.682343000
H	10.236311000	-2.280990000	17.076267000
H	9.757151000	-3.493089000	15.872337000
C	9.802312000	-8.558630000	14.924249000
H	10.809430000	-8.493889000	14.499851000
H	9.845076000	-9.272325000	15.756514000
H	9.140706000	-8.973662000	14.159929000
C	7.498829000	-7.185474000	16.380863000
H	6.789196000	-7.603895000	15.660203000
H	7.596835000	-7.910883000	17.197062000
H	7.071784000	-6.267906000	16.801047000
C	10.419701000	-6.470769000	16.997820000
H	10.186027000	-7.085853000	17.875311000
H	11.449281000	-6.694531000	16.704549000
H	10.378639000	-5.423239000	17.304288000
C	10.461221000	-6.371936000	11.788273000
H	9.624582000	-6.145474000	11.121626000
H	11.387083000	-6.209564000	11.223594000
H	10.403516000	-7.434223000	12.046123000
C	10.540949000	-3.471274000	12.833648000
H	10.809291000	-2.838259000	13.684665000
H	11.323544000	-3.359716000	12.074628000
H	9.616514000	-3.080962000	12.402694000
C	12.128321000	-5.605504000	14.194528000
H	12.303549000	-6.655589000	14.447049000
H	12.914842000	-5.301854000	13.492566000
H	12.249279000	-5.010552000	15.104894000

Complex 3 (s=2)

U	8.212164000	4.392481000	4.309040000
Si	9.417008000	7.892785000	3.970034000
Si	6.745365000	7.478184000	2.743145000
Si	11.037588000	4.127197000	2.012346000
Si	11.583871000	3.070303000	4.767838000
Si	6.719210000	1.808925000	2.048603000
Si	4.897517000	3.108752000	4.014523000
N	7.776747000	5.253234000	6.688995000
N	7.539406000	4.732042000	9.107215000
N	8.112898000	6.783328000	3.586394000
N	10.455315000	3.803665000	3.632761000
N	6.501729000	3.018074000	3.293998000

C	7.706979000	4.327591000	7.763490000
C	7.472649000	6.027792000	9.335107000
H	7.379653000	6.321421000	10.380183000
C	7.508020000	7.002147000	8.323577000
H	7.427766000	8.058812000	8.544039000
C	7.645869000	6.530746000	7.011359000
H	7.651786000	7.219923000	6.170160000
C	10.388200000	8.527498000	2.441661000
H	10.527060000	7.745142000	1.690788000
H	11.381191000	8.879699000	2.747640000
H	9.873078000	9.364968000	1.961896000
C	8.873996000	9.512660000	4.846877000
H	8.192267000	10.110373000	4.232252000
H	9.761681000	10.127376000	5.044611000
H	8.384525000	9.326693000	5.807997000
C	10.696842000	7.108735000	5.131819000
H	10.261305000	6.862099000	6.104560000
H	11.522915000	7.811103000	5.300085000
H	11.105087000	6.188858000	4.703817000
C	5.478132000	8.303694000	3.914307000
H	5.183191000	7.645985000	4.736341000
H	4.571536000	8.597725000	3.370618000
H	5.908915000	9.207910000	4.358083000
C	5.858182000	6.186673000	1.661902000
H	6.398999000	6.079210000	0.714508000
H	4.836450000	6.510636000	1.428619000
H	5.812907000	5.193737000	2.117940000
C	7.147257000	8.863507000	1.474603000
H	7.528499000	9.781909000	1.932327000
H	6.220367000	9.120300000	0.945115000
H	7.874298000	8.528660000	0.727632000
C	12.401666000	5.463880000	1.879166000
H	12.196389000	6.325716000	2.518333000
H	12.463808000	5.822474000	0.843740000
H	13.383849000	5.067435000	2.152343000
C	9.604353000	4.727899000	0.915627000
H	8.849141000	3.948034000	0.780956000
H	9.979221000	5.001848000	-0.078355000
H	9.116308000	5.606829000	1.350876000
C	11.802019000	2.618723000	1.110222000
H	12.677726000	2.229117000	1.640120000
H	12.130813000	2.921392000	0.107648000
H	11.085470000	1.800518000	0.999209000
C	13.425724000	3.521585000	4.474780000
H	13.826992000	3.148634000	3.526898000
H	14.015988000	3.068780000	5.281652000
H	13.588161000	4.603348000	4.514110000
C	11.551940000	1.163470000	4.729510000
H	10.626678000	0.769783000	5.159110000
H	12.385848000	0.759610000	5.316880000
H	11.641600000	0.784857000	3.705844000
C	11.280619000	3.637636000	6.549827000
H	11.572454000	4.684505000	6.677726000
H	11.896028000	3.034438000	7.227652000
H	10.243746000	3.535739000	6.882779000
C	6.293554000	2.459580000	0.301114000
H	5.236328000	2.739203000	0.243244000
H	6.482501000	1.690130000	-0.458222000
H	6.880277000	3.345244000	0.040493000
C	8.497897000	1.126487000	2.006882000
H	9.237123000	1.851228000	2.358900000
H	8.769982000	0.814362000	0.991231000
H	8.576116000	0.244716000	2.653314000
C	5.668724000	0.214244000	2.227943000
H	5.904707000	-0.308083000	3.160831000
H	5.920635000	-0.458630000	1.397827000
H	4.588894000	0.385299000	2.200115000
C	4.680951000	4.702260000	5.020130000
H	5.411697000	4.808337000	5.827473000
H	3.686395000	4.690890000	5.482297000
H	4.739062000	5.585632000	4.379046000
C	3.483754000	3.188753000	2.719634000
H	3.622826000	4.042810000	2.048676000
H	2.524428000	3.320389000	3.235892000
H	3.405102000	2.286751000	2.104421000
C	4.471150000	1.679097000	5.196654000
H	4.430642000	0.708805000	4.694278000
H	3.493390000	1.860994000	5.659004000
H	5.213339000	1.616164000	5.997092000
N	7.714610000	2.070465000	8.566448000
N	7.976146000	2.600529000	6.154465000
C	7.795525000	2.999153000	7.496167000
C	8.097103000	1.308671000	5.927694000
H	8.209551000	1.020803000	4.883178000
C	8.088659000	0.333711000	6.940471000
H	8.208212000	-0.719638000	6.721419000
C	7.895072000	0.797131000	8.246692000
H	7.877797000	0.107471000	9.087407000
U	7.253947000	2.933226000	10.940903000
Si	5.985221000	-0.555348000	11.178417000
Si	8.641233000	-0.244206000	12.470845000
Si	4.421248000	3.194374000	13.242097000
Si	3.913695000	4.375048000	10.530676000
Si	8.792186000	5.432008000	13.289349000
Si	10.607344000	4.139728000	11.314109000
N	7.311643000	0.502984000	11.617084000
N	5.016495000	3.562896000	11.636086000
N	8.998179000	4.250338000	12.017274000
C	4.957959000	-1.199500000	12.665425000
H	4.794868000	-0.422176000	13.416584000
H	3.975350000	-1.545892000	12.321192000
H	5.452483000	-2.042051000	13.157557000
C	6.491761000	-2.167341000	10.265649000
H	7.140759000	-2.805286000	10.875449000
H	5.588795000	-2.746089000	10.031924000
H	7.006760000	-1.968648000	9.320652000
C	4.754475000	0.307237000	10.018006000
H	5.212358000	0.562901000	9.057884000
H	3.906365000	-0.359709000	9.819508000
H	4.369615000	1.228272000	10.466178000
C	9.919749000	-1.074535000	11.314072000
H	10.277963000	-0.398315000	10.533011000
H	10.789618000	-1.430182000	11.880636000
H	9.470588000	-1.939864000	10.814218000
C	9.540573000	1.000477000	13.596117000
H	8.971334000	1.123183000	14.524729000
H	10.539174000	0.632278000	13.861572000
H	9.643701000	1.994174000	13.151583000
C	8.175497000	-1.649121000	13.695148000
H	7.770627000	-2.539362000	13.202969000
H	9.082311000	-1.954419000	14.233441000
H	7.445868000	-1.310687000	14.438049000
C	3.006366000	1.905800000	13.315822000
H	3.169904000	1.073831000	12.626526000
H	2.938915000	1.491779000	14.329995000
H	2.038827000	2.356255000	13.076460000

C	5.822529000	2.496534000	14.321313000
H	6.610012000	3.237991000	14.485698000
H	5.430797000	2.206058000	15.304193000
H	6.275327000	1.614105000	13.856832000
C	3.711092000	4.692247000	14.205042000
H	2.853792000	5.137752000	13.689528000
H	3.366079000	4.359710000	15.192585000
H	4.458250000	5.476491000	14.353679000
C	2.055474000	3.985530000	10.809474000
H	1.665852000	4.343529000	11.767839000
H	1.483897000	4.483178000	10.015768000
H	1.855639000	2.911750000	10.738005000
C	4.025595000	6.276583000	10.640287000
H	4.974137000	6.643830000	10.238776000
H	3.219408000	6.740253000	10.058403000
H	3.939335000	6.619581000	11.676741000
C	4.190475000	3.866641000	8.727343000
H	3.875526000	2.831882000	8.561348000
H	3.584759000	4.509040000	8.077209000
H	5.228005000	3.958401000	8.395204000
C	9.163562000	4.728319000	15.028200000
H	10.212412000	4.421095000	15.098522000
H	8.978863000	5.482600000	15.803537000
H	8.550980000	3.850890000	15.254754000
C	7.034669000	6.166109000	13.305309000
H	6.274726000	5.457374000	12.965370000
H	6.766269000	6.511017000	14.311304000
H	6.987268000	7.034298000	12.637852000
C	9.890992000	7.001063000	13.175355000
H	9.693320000	7.554860000	12.251707000
H	9.638749000	7.659557000	14.016976000
H	10.964867000	6.798739000	13.224063000
C	10.777602000	2.590989000	10.233424000
H	10.117428000	2.610061000	9.361958000
H	11.808479000	2.529280000	9.863593000
H	10.576080000	1.679469000	10.802109000
C	11.999506000	3.966539000	12.623312000
H	11.830975000	3.091075000	13.259048000
H	12.963634000	3.833132000	12.116475000
H	12.089084000	4.841819000	13.274983000
C	11.102546000	5.602832000	10.199414000
H	11.212435000	6.539763000	10.752115000
H	12.060806000	5.385280000	9.712099000
H	10.357194000	5.756689000	9.413976000

Complex 3 (s=3)

U	8.217622604	4.370762243	4.311009664
Si	9.445036533	7.874453804	4.022146092
Si	6.777432854	7.515952093	2.768453221
Si	11.046276088	4.119405166	2.004356199
Si	11.575613148	2.989235495	4.734630340
Si	6.704385227	1.831586178	1.984622650
Si	4.885902007	3.113327559	3.964806562
N	7.771028757	5.245897056	6.692538535
N	7.519643634	4.723879046	9.107362181
N	8.127443922	6.794042140	3.612032137
N	10.459062382	3.764945840	3.616622220
N	6.490908774	3.018676271	3.250137870
C	7.691437853	4.319190216	7.764980790
C	7.425832679	6.019040892	9.332884295
H	7.326628878	6.312062210	10.377555857
C	7.444380871	6.991170720	8.320123708
H	7.345091873	8.046784609	8.537853158
C	7.613494807	6.520424164	7.010719586
H	7.627615902	7.208428144	6.168636654
C	10.443927384	8.516896681	2.515050874
H	10.600220943	7.737290003	1.764778079
H	11.429468151	8.872008482	2.841452164
H	9.935202306	9.353800025	2.027679157
C	8.928639444	9.490797665	4.921910402
H	8.260542054	10.109993256	4.313431709
H	9.826201318	10.086518953	5.132843099
H	8.431437201	9.299183112	5.877892915
C	10.699693036	7.040877397	5.178009965
H	10.255476782	6.791773028	6.146239757
H	11.542872423	7.718938136	5.358982763
H	11.088620851	6.118138857	4.737118532
C	5.501501838	8.336375800	3.934969432
H	5.169982875	7.663840730	4.730843019
H	4.615547467	8.667459779	3.378622636
H	5.942014381	9.216848953	4.415721671
C	5.885001882	6.248956765	1.662787631
H	6.441046519	6.134814291	0.725086604
H	4.874587668	6.594951901	1.412720160
H	5.810148702	5.254723732	2.111781297
C	7.205304410	8.917389136	1.526219154
H	7.597631660	9.820888908	2.004124420
H	6.286685515	9.198847402	0.994980231
H	7.933028434	8.585392326	0.778582191
C	12.436563365	5.432392877	1.908180880
H	12.249020302	6.279474417	2.572376117
H	12.504875386	5.819568586	0.883486289
H	13.410905683	5.008969055	2.168383684
C	9.630602061	4.775902990	0.917589646
H	8.857389432	4.017104091	0.765708896
H	10.015068383	5.059510774	-0.070146149
H	9.161398586	5.656450229	1.369378426
C	11.781011710	2.619265454	1.064282871
H	12.644770271	2.195133064	1.586970819
H	12.121441489	2.942144011	0.071989802
H	11.046400974	1.821207953	0.927258772
C	13.427057231	3.403447399	4.447678685
H	13.820488874	3.039322121	3.493176810
H	14.007151915	2.923917030	5.246393424
H	13.611828993	4.480724217	4.506175526
C	11.495072900	1.084727634	4.660406352
H	10.557053309	0.708051859	5.077637741
H	12.314465240	0.646832402	5.243775584
H	11.579094605	0.723717094	3.629901923
C	11.289516644	3.527264291	6.528237996
H	11.596661173	4.567116107	6.676345182
H	11.896408863	2.901241256	7.192937009
H	10.251205263	3.434745587	6.858389565
C	6.316006697	2.519583278	0.243088682
H	5.263150880	2.813741268	0.176339851
H	6.505582330	1.762345980	-0.528206738
H	6.916825550	3.402682208	0.007402131
C	8.470883661	1.118648954	1.965541048
H	9.222059233	1.837120842	2.304700272
H	8.742612474	0.777480444	0.959187740
H	8.529764684	0.251004115	2.632833030
C	5.623894186	0.251465029	2.114258905
H	5.831178735	-0.292738737	3.041444651
H	5.880147739	-0.410451041	1.276590900
H	4.547772033	0.442118066	2.068018339
C	4.713391811	4.660603735	5.047049709

H	5.370399762	4.637628446	5.920952597
H	3.681672392	4.721912623	5.414375979
H	4.916996991	5.574115540	4.482298519
C	3.483151018	3.271273210	2.665363672
H	3.639802829	4.146033895	2.025786819
H	2.521212085	3.397343868	3.178151772
H	3.397452879	2.392962275	2.017164935
C	4.409934059	1.648344796	5.085596038
H	4.290935326	0.711503683	4.534584406
H	3.459385667	1.866055196	5.587767784
H	5.167364506	1.494194405	5.859242592
N	7.695394511	2.062943529	8.570319770
N	7.946587014	2.584959422	6.155486600
C	7.774697014	2.989648782	7.497863757
C	8.040390560	1.289793872	5.929989357
H	8.139719776	0.996759325	4.885342137
C	8.021739708	0.317639173	6.942730364
H	8.121084270	-0.737966778	6.724996680
C	7.852851731	0.788402133	8.252152478
H	7.838935957	0.100457421	9.094291503
U	7.248904912	2.938058234	10.951851816
Si	6.020717326	-0.565306296	11.240640775
Si	8.688321005	-0.207637511	12.494473348
Si	4.420867920	3.190202726	13.259170457
Si	3.890869388	4.320166018	10.528975164
Si	8.763194823	5.477057554	13.277453002
Si	10.581318731	4.194223421	11.297757521
N	7.338594634	0.514734944	11.650825111
N	5.007721255	3.544474194	11.646711816
N	8.976236292	4.289531947	12.012237826
C	5.021520611	-1.207535385	12.747629098
H	4.865550379	-0.427949875	13.497993441
H	4.035827441	-1.562139706	12.421142611
H	5.529839280	-2.044725015	13.234927260
C	6.536675198	-2.181675558	10.340657914
H	7.204109528	-2.801517803	10.949199580
H	5.638856673	-2.776761833	10.129022470
H	7.034442073	-1.989896960	9.385006137
C	4.766330174	0.268677577	10.084794364
H	5.210748574	0.518021134	9.116714330
H	3.923116391	-0.409237638	9.903478659
H	4.377435168	1.191340445	10.525872598
C	9.963673101	-1.028811591	11.327864531
H	10.295402147	-0.356326792	10.532036454
H	10.849539628	-1.360412047	11.884044637
H	9.522609155	-1.908985759	10.847089009
C	9.581448374	1.059109105	13.599882287
H	9.025886876	1.173116110	14.537886533
H	10.591971599	0.713032476	13.849372427
H	9.656116342	2.053420985	13.151025149
C	8.259805440	-1.608629515	13.736986292
H	7.867174971	-2.512083778	13.259246130
H	9.178263994	-1.890317973	14.268384498
H	7.532140155	-1.276170733	14.484476673
C	3.030282186	1.877538342	13.355788698
H	3.217002908	1.030722450	12.691026712
H	2.962690905	1.489865206	14.380344645
H	2.055855200	2.301396089	13.096604031
C	5.836645665	2.533408033	14.345604688
H	6.610282695	3.291867201	14.497012882
H	5.452355030	2.250284446	15.333550036
H	6.305260166	1.652508363	13.893896871
C	3.686626549	4.690524475	14.199324750
H	2.822775912	5.114692849	13.676818309
H	3.346398387	4.367757574	15.191725241
H	4.421351059	5.488515829	14.336099077
C	2.039500448	3.906030316	10.816464992
H	1.646324398	4.270385256	11.770981684
H	1.459245423	4.385429449	10.017786237
H	1.854654601	2.828755085	10.758241207
C	3.971474725	6.224678113	10.602986952
H	4.909351967	6.601253343	10.185341217
H	3.151885001	6.662513548	10.019848970
H	3.887832969	6.585846877	11.633466509
C	4.176495454	3.782146218	8.735294482
H	3.868914882	2.742446276	8.587059234
H	3.569858827	4.408528035	8.070698129
H	5.214830118	3.874297144	8.405112220
C	9.152154918	4.789565289	15.019066347
H	10.204980043	4.495279766	15.085619382
H	8.962884621	5.547068762	15.790177084
H	8.551267272	3.906626699	15.255203757
C	6.996683159	6.190006948	13.297206130
H	6.245485362	5.472038837	12.956997548
H	6.724862269	6.529733980	14.304018235
H	6.937852937	7.058642407	12.631186291
C	9.843569445	7.057182407	13.146847824
H	9.635890658	7.600996169	12.219519729
H	9.587491049	7.719380528	13.984347022
H	10.919723878	6.866678068	13.192796284
C	10.754250681	2.645907941	10.217047401
H	10.096012922	2.666861773	9.344018713
H	11.785529296	2.585478016	9.848351090
H	10.552591815	1.732869220	10.783259120
C	11.984049612	4.037351471	12.597359164
H	11.827306782	3.163112555	13.237633472
H	12.945922926	3.910699247	12.084590114
H	12.069934550	4.916173591	13.244824462
C	11.057005686	5.658295999	10.175688495
H	11.174945007	6.595832452	10.725747607
H	12.007982711	5.440786157	9.674252305
H	10.299837181	5.810993798	9.401496888

Complex 4 (s=5/2)

U	7.712518158	0.639857317	9.359546361
Si	10.755228601	0.955825348	10.967084712
Si	9.391632494	3.612371868	10.794266536
Si	9.654625650	0.059770041	6.384612411
Si	6.798956609	-0.868801091	6.231062636
Si	5.601370815	3.062558294	7.952060823
Si	4.306531767	1.479835710	10.166017780
N	7.348724145	-0.035404604	11.882141716
N	7.001501318	-1.753792359	13.559487542
N	9.310211695	1.857484112	10.381434197
N	8.076972583	-0.104541082	7.252573168
N	5.790868129	1.761368061	9.189593150
C	7.246221454	-1.348890271	12.267718780
C	6.777652992	-0.792472564	14.453107575
H	6.533482671	-1.129410831	15.454868683
C	6.856030492	0.565616394	14.141145416
H	6.690741450	1.329290074	14.890044996
C	7.180529919	0.887650913	12.823895182
H	7.307169443	1.920192145	12.511697009
C	10.893739687	-0.675521746	10.010576197
H	9.980510462	-1.276150624	9.955651303
H	11.630299384	-1.298685108	10.528874091

H	11.265751823	-0.502070674	8.999467173
C	12.407263350	1.832146047	10.647430433
H	12.537758989	2.090428995	9.592987084
H	13.209036734	1.134665032	10.917935259
H	12.551357257	2.737182550	11.242521471
C	10.683504446	0.516509804	12.810682155
H	10.548548372	1.388166335	13.454024104
H	11.629703001	0.040347119	13.092043582
H	9.882071852	-0.194983295	13.023321978
C	10.481282006	4.582605125	9.586908425
H	11.535815844	4.307184242	9.656887882
H	10.399994559	5.650926147	9.818728277
H	10.167103123	4.444973531	8.548213391
C	10.042639046	3.934519631	12.552221403
H	9.388298149	3.509579188	13.320664558
H	10.046223693	5.021397841	12.697464154
H	11.059669564	3.582361168	12.738530954
C	7.673944840	4.413787528	10.765448601
H	7.499755036	4.905078861	9.805758672
H	7.631845086	5.188846457	11.538539519
H	6.847586411	3.719420192	10.935481189
C	10.640091273	1.524481336	7.081613462
H	10.306357704	2.444691467	6.591098961
H	11.700197348	1.390151279	6.838038466
H	10.558400065	1.681917918	8.158952723
C	10.653802785	-1.554523787	6.485724954
H	10.711833420	-1.978699040	7.490860096
H	11.678466155	-1.375615309	6.140499771
H	10.219056158	-2.312283382	5.826938967
C	9.519706089	0.455785127	4.534085392
H	9.119551778	-0.361146010	3.928812984
H	10.541011829	0.646442398	4.181931162
H	8.933417385	1.356422580	4.333318719
C	6.248340803	0.204473031	4.765013581
H	6.353905314	1.274692741	4.948821711
H	5.194035040	0.007389960	4.542218846
H	6.820832268	-0.039813709	3.867122559
C	7.325781666	-2.521189860	5.441168223
H	8.122773404	-2.394715968	4.703437458
H	6.451675044	-2.907704097	4.902810807
H	7.638676235	-3.300115486	6.141770326
C	5.273519579	-1.257848500	7.292499062
H	5.449116995	-2.051315388	8.024819520
H	4.478853575	-1.608664440	6.624133380
H	4.896852272	-0.374949069	7.815020849
C	4.875479861	4.681061727	8.630473465
H	3.812866015	4.567936332	8.866571715
H	4.943506655	5.433365505	7.835194673
H	5.380276327	5.078205019	9.511566814
C	7.320589908	3.392124593	7.214805788
H	8.099044037	3.580152912	7.960934596
H	7.265736452	4.287922719	6.585715641
H	7.642730262	2.563121865	6.578592915
C	4.444569769	2.601398314	6.517728535
H	4.783514147	3.105692061	5.605686255
H	3.424571625	2.941157625	6.713636832
H	4.407649601	1.531398741	6.309393040
C	4.139667892	2.705269987	11.603806654
H	4.967848808	2.639466267	12.315103957
H	3.218515296	2.483408721	12.155368630
H	4.075925847	3.740025296	11.256964834
C	4.301712549	-0.269983057	10.908417477
H	4.853733322	-1.007730756	10.319301908
H	3.263569447	-0.614850516	10.957275883
H	4.692817400	-0.267338759	11.927669480
C	2.705026036	1.599783259	9.157048220
H	2.490943146	2.608748056	8.797275955
H	1.879920169	1.310547675	9.818752090
H	2.696077120	0.920985905	8.299914429
N	7.266757764	-3.653827614	11.654122943
N	7.643134554	-1.930744469	9.984598357
C	7.387730859	-2.337643673	11.276554447
C	7.830911513	-2.895187468	9.082853865
H	8.081963254	-2.556133021	8.083834425
C	7.709944769	-4.250900421	9.384143049
H	7.842369259	-5.013277087	8.627512189
C	7.398754679	-4.574473787	10.705741532
H	7.252168348	-5.605165545	11.014557203
U	6.948269791	-4.337635747	14.161063118
Si	3.873570054	-4.588657854	12.733204785
Si	5.118109746	-7.310756736	12.790911564
Si	5.082427324	-3.874823675	17.263878571
Si	7.925914704	-2.897757153	17.263380086
Si	9.089353220	-6.772870817	15.370202969
Si	10.353748701	-5.154810834	13.166864482
N	5.299359304	-5.567524109	13.211479945
N	6.603172669	-3.664546628	16.303440386
N	8.889343800	-5.440805208	14.173445866
C	4.016025628	-2.901019530	13.606975908
H	4.470866703	-2.148851222	12.962021027
H	2.997343548	-2.565226932	13.831287265
H	4.538868625	-2.895195406	14.570512956
C	2.203097711	-5.325512831	13.245508688
H	2.134209946	-5.513866594	14.319759142
H	1.424286916	-4.598847691	12.984814279
H	1.964006963	-6.254057504	12.720988728
C	3.751587290	-4.186093141	10.883213294
H	3.525413229	-5.058791623	10.267698130
H	2.937315269	-3.465483906	10.743780380
H	4.666487657	-3.724830501	10.502497780
C	4.108109349	-8.263455704	14.079929133
H	3.073241854	-7.917378017	14.137741747
H	4.089561157	-9.323977183	13.803460479
H	4.541314483	-8.191157392	15.081503441
C	4.290260625	-7.576015299	11.099143012
H	4.844379056	-7.098300537	10.284919146
H	4.289569519	-8.654788101	10.903648002
H	3.251664018	-7.240810616	11.048201235
C	6.792999132	-8.178100472	12.651379165
H	7.199023606	-8.414073837	13.635300121
H	6.640411931	-9.128486936	12.127542902
H	7.550393595	-7.613647210	12.100451144
C	4.075363860	-5.333636761	16.598215926
H	4.459086159	-6.268389741	17.018847809
H	3.035185013	-5.227788081	16.926217977
H	4.080496351	-5.436334718	15.511840964
C	4.027066911	-2.293890768	17.263404958
H	3.700128507	-1.969145803	16.273126996
H	3.126256418	-2.478307981	17.860326420
H	4.560962305	-1.462481342	17.732765069
C	5.348864894	-4.295612723	19.095433527
H	5.761889854	-3.476277534	19.688826436
H	4.358552007	-4.523927306	19.508258458
H	5.974367749	-5.179987500	19.243419003
C	8.576219567	-3.969172274	18.691292396
H	8.476435788	-5.040772608	18.511582743

H	9.639409687	-3.756697555	18.848877676
H	8.056586559	-3.735508239	19.623399490
C	7.429384517	-1.252195829	18.084783300
H	6.661444609	-1.384123950	18.851925208
H	8.322433567	-0.864606303	18.590056554
H	7.087567235	-0.472771717	17.398482742
C	9.394077293	-2.500495854	16.126021542
H	9.176304980	-1.724866473	15.386269849
H	10.208948872	-2.122757492	16.754198858
H	9.767209168	-3.387774756	15.607333644
C	9.771945833	-8.386624355	14.637857640
H	10.836590661	-8.287606825	14.404297324
H	9.689371957	-9.163422689	15.407750211
H	9.260692347	-8.745338266	13.743904755
C	7.377942138	-7.080404821	16.145802187
H	6.539085600	-7.066994940	15.439935301
H	7.374562283	-8.077643051	16.600650142
H	7.169842655	-6.354544560	16.935666966
C	10.280061299	-6.372465147	16.794039026
H	9.960638798	-6.913729863	17.692035354
H	11.295957260	-6.701791729	16.563092316
H	10.319948563	-5.311369511	17.044593870
C	10.452845079	-6.350115875	11.698939494
H	9.605211078	-6.249753177	11.015564228
H	11.361994347	-6.138849267	11.123988413
H	10.502265471	-7.392144197	12.025262994
C	10.388693979	-3.385270689	12.478508600
H	9.943974478	-2.645722729	13.149813333
H	11.438388492	-3.102344486	12.346230692
H	9.907354354	-3.309856052	11.501785514
C	11.977030605	-5.334446931	14.133303538
H	12.180351617	-6.355795006	14.463320696
H	12.792418132	-5.045028252	13.459733926
H	12.021032222	-4.677807287	15.006706883

Complex 4 (s=3/2)

U	7.696128480	0.635121709	9.355361098
Si	10.739669731	0.921410834	10.967822386
Si	9.391259954	3.586280255	10.816122614
Si	9.639845200	0.067943713	6.377485981
Si	6.781096348	-0.850477270	6.218553944
Si	5.611938484	3.091342361	7.954921026
Si	4.296992818	1.491027280	10.146276823
N	7.324184079	-0.042413557	11.870576547
N	6.981837092	-1.768375955	13.544403874
N	9.300706614	1.835849229	10.385342700
N	8.060831090	-0.094717965	7.243691986
N	5.787812660	1.777260312	9.180628887
C	7.223814501	-1.358199028	12.252046667
C	6.755243923	-0.808970723	14.440620579
H	6.513795161	-1.149757697	15.441848806
C	6.827958169	0.549230421	14.131644567
H	6.659633236	1.310587892	14.882243865
C	7.152716363	0.876535545	12.814600713
H	7.276916380	1.910693414	12.506648129
C	10.876576352	-0.705638811	10.003831304
H	9.960754159	-1.301639505	9.944599965
H	11.609763602	-1.333045116	10.522114910
H	11.251878912	-0.530009645	8.994332566
C	12.396714202	1.792975289	10.660400038
H	12.532292588	2.058565117	9.608404134
H	13.194122931	1.089497637	10.928319833
H	12.543288891	2.692827971	11.262732337
C	10.656559798	0.469100814	12.807681191
H	10.499837077	1.333044587	13.456298508
H	11.606913983	0.005733635	13.096333622
H	9.864542327	-0.257281745	13.004726690
C	10.490032481	4.560794026	9.620441858
H	11.543205275	4.280943401	9.692727470
H	10.411693610	5.627677803	9.859814657
H	10.179548843	4.431933545	8.579535392
C	10.038000808	3.890473563	12.578850661
H	9.377137271	3.464854714	13.341298766
H	10.048520322	4.976264843	12.731884488
H	11.051630832	3.529765183	12.767107584
C	7.677733220	4.397369275	10.788061403
H	7.517423735	4.911069677	9.837623080
H	7.630021541	5.154892857	11.577999208
H	6.846047034	3.703418402	10.931580094
C	10.634049657	1.520727882	7.086123640
H	10.299077283	2.448843921	6.611747986
H	11.691673890	1.386652359	6.831839154
H	10.561592062	1.662472241	8.166221502
C	10.630585133	-1.552168419	6.467358270
H	10.685086686	-1.983719874	7.469548541
H	11.656605843	-1.375652352	6.124966831
H	10.193176215	-2.303154016	5.802694182
C	9.506061783	0.478303207	4.530034540
H	9.101388828	-0.332426502	3.919419559
H	10.527986661	0.666375447	4.178320057
H	8.923921300	1.383096817	4.335885229
C	6.233269834	0.230682121	4.757435234
H	6.345815252	1.299528617	4.944901037
H	5.177307747	0.040684205	4.536267719
H	6.802313710	-0.013866561	3.857405277
C	7.302155489	-2.501338834	5.422138480
H	8.097972983	-2.374145261	4.683240879
H	6.426089853	-2.883878950	4.884121855
H	7.614543636	-3.283242141	6.119588274
C	5.254866081	-1.238191682	7.279197134
H	5.431112797	-2.027191785	8.016218802
H	4.462475539	-1.594932820	6.611268552
H	4.874585022	-0.353304661	7.795701646
C	4.893039550	4.708109564	8.644751725
H	3.828953533	4.598361907	8.875994245
H	4.967452984	5.466394632	7.855736276
H	5.396399828	5.095880598	9.530865908
C	7.336747806	3.413076308	7.228398235
H	8.113997528	3.580547149	7.980691958
H	7.295597924	4.318563141	6.612339607
H	7.651282296	2.589326193	6.581629863
C	4.457058881	2.651981309	6.511951507
H	4.806149704	3.158006524	5.604680289
H	3.440031539	3.002313052	6.704885299
H	4.408678322	1.583869311	6.296440369
C	4.123213126	2.706480744	11.591684790
H	4.944077108	2.631857756	12.310514403
H	3.195760675	2.484699913	12.132644171
H	4.067284911	3.743925862	11.251609561
C	4.284606895	-0.264435692	10.877185435
H	4.846741832	-0.998574932	10.293207649
H	3.246520415	-0.611619889	10.907718963
H	4.660754021	-0.266908008	11.902111277
C	2.702434655	1.623303071	9.128083174
H	2.493372599	2.636525099	8.777323326
H	1.872137559	1.329268378	9.781076257

H	2.697908073	0.953652546	8.263792261
N	7.242819902	-3.658683344	11.638235984
N	7.623312103	-1.935285868	9.968947939
C	7.365812866	-2.343418584	11.260114497
C	7.810415420	-2.898860487	9.065999041
H	8.060957034	-2.559791752	8.066880115
C	7.691397106	-4.254437971	9.367904187
H	7.826762763	-5.017096160	8.612020525
C	7.378947045	-4.577927198	10.689506374
H	7.234579554	-5.609294715	10.997186431
U	6.943945355	-4.343242380	14.158063741
Si	3.879977332	-4.600303987	12.719416543
Si	5.159781396	-7.312074916	12.759504894
Si	5.124178351	-3.856004545	17.254398890
Si	7.961926804	-2.855704495	17.247537049
Si	9.082472329	-6.792384228	15.435654786
Si	10.313322735	-5.186593749	13.200145498
N	5.317969410	-5.568232677	13.190803932
N	6.643979644	-3.641453862	16.295224380
N	8.863914716	-5.474795321	14.225954537
C	3.999080843	-2.913868483	13.599218170
H	4.424819815	-2.151230403	12.946331451
H	2.977296197	-2.602906469	13.844144155
H	4.539803152	-2.894841915	14.552490237
C	2.221674478	-5.366315572	13.226873182
H	2.160556623	-5.577682724	14.297291863
H	1.432679667	-4.644443191	12.984279281
H	1.993045565	-6.286513533	12.683293845
C	3.754252226	-4.193364566	10.871370307
H	3.559229772	-5.069303729	10.249946880
H	2.916859393	-3.499304153	10.733497408
H	4.654577464	-3.699201388	10.497700259
C	4.140683913	-8.272912102	14.034935837
H	3.100221426	-7.942051435	14.075805255
H	4.141799947	-9.334183425	13.760430431
H	4.557236897	-8.192881451	15.043034901
C	4.354405903	-7.581760047	11.058366200
H	4.906380108	-7.090830671	10.250700957
H	4.372652464	-8.659364426	10.857455591
H	3.310673631	-7.263666311	11.001384394
C	6.845902569	-8.160933962	12.651348473
H	7.208920808	-8.428817245	13.644180244
H	6.724074854	-9.093026240	12.088200691
H	7.623010472	-7.571547455	12.157896509
C	4.114573249	-5.311678551	16.581161602
H	4.485361397	-6.246698766	17.012379146
H	3.071699302	-5.194373713	16.896661840
H	4.127948733	-5.424667948	15.495511083
C	4.067108695	-2.276141105	17.255432902
H	3.742343622	-1.949725528	16.264859131
H	3.164850373	-2.462551729	17.849564013
H	4.598739210	-1.444982509	17.727593949
C	5.388121908	-4.282446793	19.084427170
H	5.797717799	-3.462698846	19.679662144
H	4.398180504	-4.515243507	19.495631760
H	6.017229518	-5.164457736	19.231219351
C	8.609873653	-3.911066496	18.688306248
H	8.500692215	-4.984139530	18.524276118
H	9.675110101	-3.704578887	18.839757835
H	8.094861950	-3.659619459	19.618465441
C	7.456811244	-1.205385867	18.054584742
H	6.684851178	-1.332866254	18.818564816
H	8.346785246	-0.814207461	18.562622947
H	7.119401480	-0.430248091	17.361261473
C	9.430268255	-2.461525654	16.110674872
H	9.208463611	-1.700448118	15.357114299
H	10.238176919	-2.065536498	16.736713254
H	9.814136606	-3.353006752	15.607913093
C	9.772153271	-8.409514975	14.716606623
H	10.832245058	-8.304264795	14.465485560
H	9.708612842	-9.174646539	15.499921246
H	9.251560335	-8.788001594	13.836302278
C	7.380030271	-7.103212890	16.222941413
H	6.550189326	-7.137408853	15.508244146
H	7.392985059	-8.074861695	16.729549782
H	7.153866265	-6.340526125	16.972537920
C	10.285446206	-6.363902530	16.840780194
H	9.976590317	-6.889803643	17.751486831
H	11.299957311	-6.694490670	16.605300022
H	10.324211615	-5.298456528	17.071664461
C	10.413426136	-6.390763038	11.739433724
H	9.565720697	-6.298702601	11.054821771
H	11.321646699	-6.179064621	11.163027406
H	10.467862071	-7.430668830	12.072020038
C	10.315247352	-3.416722339	12.503145505
H	9.740715380	-2.704898504	13.101935492
H	11.349516348	-3.057545927	12.497257350
H	9.950561676	-3.382259671	11.474448217
C	11.948807465	-5.345651201	14.148997348
H	12.163975168	-6.362775912	14.484563987
H	12.753446873	-5.055221264	13.462884119
H	11.998169119	-4.681661285	15.016500896

Complex 4 (s=1/2)

U	7.695301000	0.640642000	9.359735000
Si	10.738650000	0.925389000	10.977836000
Si	9.394924000	3.591920000	10.796276000
Si	9.660485000	0.068962000	6.390632000
Si	6.801610000	-0.840751000	6.219885000
Si	5.597829000	3.074598000	7.949934000
Si	4.291613000	1.488498000	10.156109000
N	7.319642000	-0.039148000	11.874125000
N	6.979734000	-1.767120000	13.545237000
N	9.305005000	1.837930000	10.382831000
N	8.078550000	-0.089544000	7.251904000
N	5.780197000	1.768136000	9.184384000
C	7.218401000	-1.355333000	12.252919000
C	6.755902000	-0.808448000	14.443390000
H	6.516607000	-1.150692000	15.444654000
C	6.828902000	0.549927000	14.136726000
H	6.662628000	1.310213000	14.888842000
C	7.151678000	0.878862000	12.819367000
H	7.277157000	1.913198000	12.512437000
C	10.866653000	-0.707628000	10.022906000
H	9.946151000	-1.296028000	9.958620000
H	11.590252000	-1.340206000	10.548089000
H	11.249689000	-0.538606000	9.015243000
C	12.400222000	1.787605000	10.668925000
H	12.540899000	2.043349000	9.615186000
H	13.194195000	1.083945000	10.946371000
H	12.547288000	2.692294000	11.263881000
C	10.652014000	0.485368000	12.820703000
H	10.504126000	1.355277000	13.463515000
H	11.598640000	0.015630000	13.111401000
H	9.853917000	-0.232542000	13.024209000
C	10.494980000	4.558077000	9.595397000

H	11.545728000	4.267228000	9.660193000
H	10.429239000	5.625330000	9.836830000
H	10.176478000	4.433972000	8.556324000
C	10.039680000	3.907786000	12.557682000
H	9.377215000	3.488413000	13.322198000
H	10.051934000	4.994567000	12.703209000
H	11.052464000	3.546595000	12.749591000
C	7.681799000	4.403980000	10.763002000
H	7.511542000	4.896655000	9.803350000
H	7.643894000	5.179276000	11.536125000
H	6.850374000	3.715396000	10.932648000
C	10.654843000	1.521551000	7.098003000
H	10.316321000	2.450063000	6.626764000
H	11.711820000	1.390295000	6.839630000
H	10.584450000	1.659984000	8.178447000
C	10.648327000	-1.552943000	6.483894000
H	10.696853000	-1.986156000	7.485678000
H	11.676393000	-1.378124000	6.146831000
H	10.212781000	-2.302276000	5.816090000
C	9.533998000	0.477891000	4.541970000
H	9.130742000	-0.332219000	3.929628000
H	10.557638000	0.664466000	4.194479000
H	8.954132000	1.383640000	4.345433000
C	6.259494000	0.243699000	4.758932000
H	6.358632000	1.312757000	4.952695000
H	5.207934000	0.043894000	4.525659000
H	6.840568000	0.009754000	3.863850000
C	7.322499000	-2.490141000	5.419641000
H	8.119075000	-2.361192000	4.681903000
H	6.446727000	-2.870595000	4.879671000
H	7.634149000	-3.274546000	6.114637000
C	5.269920000	-1.230315000	7.272897000
H	5.439360000	-2.029160000	8.000690000
H	4.476588000	-1.573207000	6.598830000
H	4.894465000	-0.349399000	7.799707000
C	4.878260000	4.692817000	8.635500000
H	3.815569000	4.582668000	8.872608000
H	4.947901000	5.447681000	7.842784000
H	5.385743000	5.085135000	9.517289000
C	7.318425000	3.401942000	7.214869000
H	8.097167000	3.586577000	7.961473000
H	7.264584000	4.299813000	6.588563000
H	7.639935000	2.574300000	6.576724000
C	4.439611000	2.624040000	6.513295000
H	4.781599000	3.130487000	5.603595000
H	3.421267000	2.968208000	6.710089000
H	4.397307000	1.555161000	6.300102000
C	4.126680000	2.709389000	11.597824000
H	4.952230000	2.637481000	12.311518000
H	3.202764000	2.489955000	12.145744000
H	4.068704000	3.745533000	11.254154000
C	4.277044000	-0.265007000	10.890188000
H	4.827455000	-1.001973000	10.298667000
H	3.237068000	-0.605078000	10.933937000
H	4.665697000	-0.269517000	11.910378000
C	2.693299000	1.619525000	9.143640000
H	2.484019000	2.630835000	8.787693000
H	1.865644000	1.330829000	9.802399000
H	2.683499000	0.944322000	8.283694000
N	7.234244000	-3.654559000	11.635953000
N	7.609884000	-1.929699000	9.966900000
C	7.356344000	-2.339389000	11.258296000
C	7.796396000	-2.893235000	9.063348000
H	8.047090000	-2.553529000	8.064588000
C	7.677022000	-4.248640000	9.364421000
H	7.810598000	-5.010664000	8.607545000
C	7.367423000	-4.573403000	10.686524000
H	7.223535000	-5.604916000	10.993857000
U	6.941030000	-4.342719000	14.156963000
Si	3.873638000	-4.597520000	12.725737000
Si	5.153651000	-7.309222000	12.758056000
Si	5.127942000	-3.859631000	17.258036000
Si	7.965639000	-2.859704000	17.246554000
Si	9.079731000	-6.795619000	15.428710000
Si	10.307536000	-5.187609000	13.193342000
N	5.312945000	-5.566101000	13.191958000
N	6.645733000	-3.643911000	16.295729000
N	8.859639000	-5.476321000	14.221022000
C	3.995761000	-2.912708000	13.608318000
H	4.420012000	-2.148940000	12.955838000
H	2.974837000	-2.601703000	13.856731000
H	4.539004000	-2.895968000	14.560232000
C	2.216617000	-5.364086000	13.236357000
H	2.158177000	-5.577414000	14.306519000
H	1.427167000	-4.641609000	12.997049000
H	1.986453000	-6.283208000	12.691607000
C	3.742745000	-4.188056000	10.878641000
H	3.542192000	-5.062685000	10.257085000
H	2.907227000	-3.490977000	10.744655000
H	4.643245000	-3.696667000	10.501838000
C	4.137133000	-8.272272000	14.033850000
H	3.096763000	-7.941477000	14.077495000
H	4.137654000	-9.333033000	13.757374000
H	4.555793000	-8.194148000	15.041228000
C	4.344601000	-7.575409000	11.058095000
H	4.894070000	-7.081752000	10.250397000
H	4.363519000	-8.652474000	10.854341000
H	3.300382000	-7.258304000	11.004434000
C	6.839590000	-8.157766000	12.644918000
H	7.203489000	-8.429333000	13.636446000
H	6.717196000	-9.087765000	12.078459000
H	7.616289000	-7.566536000	12.153043000
C	4.116666000	-5.314244000	16.585017000
H	4.487743000	-6.249810000	17.014792000
H	3.074325000	-5.196810000	16.902231000
H	4.128268000	-5.426334000	15.499251000
C	4.071083000	-2.279662000	17.263865000
H	3.744721000	-1.951211000	16.274496000
H	3.169787000	-2.467266000	17.859080000
H	4.603495000	-1.449507000	17.736912000
C	5.395856000	-4.288811000	19.086854000
H	5.806847000	-3.470002000	19.682405000
H	4.406749000	-4.522078000	19.499796000
H	6.025185000	-5.171102000	19.230971000
C	8.616041000	-3.916525000	18.685145000
H	8.505503000	-4.989405000	18.520794000
H	9.681814000	-3.711058000	18.834179000
H	8.103424000	-3.665099000	19.616639000
C	7.462241000	-1.210048000	18.056085000
H	6.692924000	-1.338643000	18.822542000
H	8.353584000	-0.818452000	18.561386000
H	7.121781000	-0.434745000	17.364453000
C	9.432149000	-2.464962000	16.107510000
H	9.209291000	-1.703831000	15.354316000
H	10.240920000	-2.068933000	16.732406000
H	9.815373000	-3.356351000	15.604094000

C	9.767796000	-8.411951000	14.706334000
H	10.827532000	-8.306837000	14.453653000
H	9.705245000	-9.178066000	15.488774000
H	9.245686000	-8.789197000	13.826396000
C	7.378680000	-7.107110000	16.218601000
H	6.547640000	-7.140275000	15.505280000
H	7.392408000	-8.079337000	16.724075000
H	7.153968000	-6.345256000	16.969484000
C	10.285266000	-6.369375000	16.832334000
H	9.977302000	-6.895912000	17.742975000
H	11.299171000	-6.700507000	16.595042000
H	10.325211000	-5.304192000	17.064239000
C	10.404267000	-6.389202000	11.730325000
H	9.555332000	-6.295328000	11.047464000
H	11.311555000	-6.177043000	11.152632000
H	10.458628000	-7.429744000	12.060909000
C	10.309258000	-3.416828000	12.498847000
H	9.739852000	-2.703974000	13.101349000
H	11.344512000	-3.060544000	12.487911000
H	9.939505000	-3.380405000	11.472061000
C	11.944696000	-5.349014000	14.138917000
H	12.159827000	-6.366717000	14.472734000
H	12.748142000	-5.058342000	13.451500000
H	11.996449000	-4.686206000	15.007183000

References

(1) R. A. Andersen, *Inorg. Chem.* 1979, **18**, 1507–1509.
(2) D. E. Bergbreiter and J. M. Killough, *J. Am. Chem. Soc.* 1978, **100**, 2126–2134.
(3) D. K. Modder, C. T. Palumbo, I. Douair, F. Fadaei-Tirani, L. Maron and M. Mazzanti, *Angew. Chem. Int. Ed.* 2021, **60**, 3737–3744.
(4) G. A. Bain and J. F. Berry, *J. Chem. Educ.* 2008, **85**, 532–536.
(5) D. Gatteschi, R. Sessoli and J. Villain, *Molecular Nanomagnets*, Oxford University Press, Oxford, **2006**.
(6) **CrysAlisPro** (Rigaku, V1.171.41.118a, 2021)
(7) G. M. Sheldrick, ShelXT-Integrated space-group and crystal-structure determination, *Acta Cryst.* 2015, **A71**, 3–8.
(8) O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.* 2009, **42**, 339–341.
(9) G. M. Sheldrick, Crystal structure refinement with ShelXL, *Acta Cryst.* 2015, **C71**, 3–8.
(10) D. J. Berg, J. M. Boncella and R. A. Andersen, *Organometallics* 2002, **21**, 4622–4631.
(11) S. Demir, J. M. Zadrozny, M. Nippe and J. R. Long, *J. Am. Chem. Soc.* 2012, **134**, 18546–18549.
(12) Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
(13) (a) A. D. Becke, *J. Chem. Phys*. 1993, **98**, 5648–5652; (b) K. Burke, K., J. P. Perdew and W. Yang, W. in Electronic Density Functional Theory: Recent Progress and New Directions, Eds: J. F. Dobson, G. Vignale, M. P. Das, Plenum: New York, 1998.
(14) (a) A. Moritz, X. Cao and M. Dolg, *Theor. Chem. Acc*. 2007, **118**, 845–854; (b) A. Hollwarth, M. Bohme, S. Dapprich, A. W. Ehlers, A. Gobbi, V. Jonas, K. F. Kohler, R. Stegmann, A. Veldkamp and G. Frenking *Chem. Phys*. *Lett.* 1993, **208**, 237–240.
(15) (a) P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta* 1973, **28**, 213–222; (b) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys*. 1972, **56**, 2257–2261.