Electronic Supplementary Information for

Redox-induced reversible P-P coupling in a uranium complex

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Contents

1. Experimental Procedures

General information: All manipulations were performed under an Ar atmosphere using standard Schlenk techniques or in a glovebox with an atmosphere <1 ppm O_2/H_2O. Commercially available chemicals were used as received without further purification. The solvents were obtained by passing through a Solve Purer G5 (MIKROUNA) solvent purification system and further dried over 4 Å molecular sieves. Benzene-d_6 and tetrahydrofuran-d_8 were dried over Na/K and stored under an Ar atmosphere prior to use. Nuclear magnetic resonance (NMR) spectroscopy was performed using a Bruker AVIII-400 (^{1}H 400 MHz; ^{13}C{^{1}H} 101 MHz; ^{31}P{^{1}H} 162 MHz) spectrometer at room temperature (RT). The ^{1}H and ^{13}C{^{1}H} NMR chemical shifts (δ) are relative to tetramethylsilane, and ^{31}P{^{1}H} NMR chemical shifts are relative to 85% H_3PO_4. Absolute values of the coupling constants are provided in Hertz (Hz). Multiplicities are abbreviated as singlet (s), doublet (d), triplet (t), multiplet (m), and broad (br). Magnetic measurements were performed on crystalline samples using a Quantum Design SQUID magnetometer at temperatures ranging from 1.8 K to 300 K. The sample was added to a pre-weighed SQUID capsule in a glovebox. The capsule was then sealed, weighed, and transferred to the SQUID cavity for the magnetic measurement. All magnetic data were corrected for the diamagnetic contributions of the sample holder and of the core diamagnetism of the samples using Pascal's constant. HRMS was measured on an Agilent system using ESI-TOF (electrospray ionization-time of flight) mass spectrometer. Elemental analyses (C, H, N) were performed on a Vario EL III elemental analyzer at the Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences.

Bis(2-aminophenyl)amine and UCl_4 were prepared according to previously reported procedures.[1,2]

Synthesis of compound 1

A solution of $^{i}Pr_2PCl$ (305.2 mg, 2.0 mmol, 2 equiv.) in THF (10 mL) was added slowly to a solution of bis(2-aminophenyl)amine (199.2 mg, 1.0 mmol, 1 equiv.) and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (304.5 mg, 2.0 mmol, 2 equiv.) in THF (10 mL). The mixture was stirred vigorously at RT for 3 h, resulting in a white suspension. The precipitate, 1,8-Diazabicyclo[5.4.0]undec-7-ene hydrogen chloride, was then filtered out through celite, washed with THF (5 mL × 3). The solvent was removed, the remaining solid was washed with hexane (3 mL × 3) and dried *in vacuo* to produce a white solid **1** (yield: 85.9 mg, 20%). ^{1}H NMR (400 MHz, benzene-d_6, ppm): δ: 7.67 (m, 2H, C*H*), 6.98 (t, 2H, C*H*), 6.67 (m, 4H, C*HCH*), 4.66 (s, 1H, N*H*), 4.05 (s, 2H, N*H*P$^{i}Pr_2$), 1.50 (m, 4H, C*H*$(CH_3)_2$), 0.95 (m, 24H, CH(C*H*$_3)_2$). $^{31}P\{^{1}H\}$ NMR (162 MHz, benzene-d_6, ppm): δ: 46.24. $^{13}C\{^{1}H\}$ NMR (126 MHz, benzene-d_6, ppm): δ: 16.86 (d, *J* = 8.1 Hz, 4C, CH(*C*$H_3)_2$), 18.65 (d, *J* = 19.9 Hz, 4C, *C*H$(CH_3)_2$), 26.64 (d, *J* = 12.8 Hz, 4C, CH(*C*$H_3)_2$), 116.20 (d, *J* = 20.7 Hz, 2C, $^{i}Pr_2$PNH*C*H), 118.90 (d, *J* = 3.6 Hz, 2C, NHCH*C*H), 121.80 (s, 2C, $^{i}Pr_2$PNHCHCH*C*H), 124.14 (s, 2C, NHCHCH*C*H), 131.46 (d, *J* = 2.8 Hz, 2C, NH*C*H), 141.42 (d, *J* = 15.1 Hz, 2C, $^{i}Pr_2$PNHCH*C*H). Anal. Calcd for $C_{48}H_{72}N_6P_4U$: C, 66.80; H, 9.11; N, 9.74; Found: C, 66.33; H, 9.11; N, 9.53. HRMS (ESI) calcd for **1** $[M + H]^+$ 432.2692, found 432.2679.

Synthesis of complex 2

Method A. A 1.0 M solution of KHMDS in THF (1.0 M, 0.15 mL, 0.15 mmol, 6 equiv.)

was added dropwise at -30 ºC to a precooled solution of compound **1** (21.6 mg, 0.05 mmol, 2 equiv.) in THF (2 mL). The mixture was warmed to RT and stirred for 3 h to produce a clear yellow solution. Then a solution of UCl_4 (9.5 mg, 0.025 mmol, 1 equiv.) THF (4 mL) was added slowly, resulting in an immediate changed of color from yellow to dark brown. The solution was stirred vigorously at RT for 4 h before being dried *in vacuo* to afford the product as a dark brown solid. The product was then dissolved in Et_2O and stored at RT for one week, finally yielding complex **2** as clear brown crystals. Yield: 8.5 mg, 29%. ***Method B.*** A suspension of KC_8 (12.8 mg, 0.095 mmol, 2 equiv.) in THF (2 mL) was added to a solution of complex **3** (51.5 mg, 0.047 mmol, 1 equiv.) in THF (2 mL) and stirred for 4 h, during which time the golden color of the KC_8 faded. The solution was filtered, extracted with Et_2O , and stored at RT for one week, ultimately yielding complex **2** as dark brown crystals. Yield: 12.0 mg, 22%. ^{1}H NMR (400 MHz, THF-d_8, ppm): δ: 56.35 (s, 4H), 25.12 (s, 4H), 10.05 (s, 4H), 3.53 (THF), 3.48 (s, 4H), 1.67 (THF), 1.62 (s, 4H), 1.18 (s, 24H), -2.53 (s, 4H), -12.88 (s, 24H). ^{31}P{^{1}H} NMR (162 MHz, THF-d_8, ppm): δ: -474.56. Anal. Calcd for $C_{48}H_{72}K_2N_6P_4U$: C, 49.14; H, 6.19; N, 7.16; Found: C, 46.36; H, 6.59; N, 6.70. Satisfactory elemental analysis could not be obtained despite multiple attempts on crystalline samples from different batches, which probably due to the high sensitivity or incomplete combustion.

Synthesis of complex 3

A 2.4 M solution of ^{n}BuLi in hexane (2.4 M, 1.25 mL, 3.0 mmol, 6 equiv.) was added dropwise at -30 ºC to a precooled solution of compound **1** (431.5 mg, 1.0 mmol, 2 equiv.) in THF (5 mL), the mixture was warmed to RT and stirred for 3 h to generate a yellow

solution. Then a solution of UCl_4 (190 mg, 0.5 mmol, 1 equiv.) in THF (8 mL) was added slowly, resulting in an immediate color change from yellow to brown. The solution was stirred vigorously at RT for 4 h and then dried *in vacuo* to produce a brown solid. The product was dissolved in toluene, then stored at -30 ºC for two days, yielding complex **3** as brown crystals. Yield: 160.0 mg, 29%. ^{1}H NMR (400 MHz, benzene-d_6, ppm): δ: 66.18 (s, 1H), 43.70 (s, 1H), 39.35 (s, 1H), 33.46 (s, 1H), 30.11 (s, 1H), 25.19 (s, 3H), 10.59 (s, 1H), 3.55 (THF), 1.76 (THF), 1.29 (Hex), 0.87 (Hex), -2.09 (s, 1H), -2.25 (s, 1H), -8.93 (s, 1H), -10.17 (s, 3H), -11.4 (s, 3H), -13.05 (s, 3H), -15.50 (s, 3H), -20.25 (s, 3H), -24.28 (s, 3H), -24.47 (s, 1H), -26.49 (s, 1H), -28.21 (s, 3H), -59.41 (s, 1H). ^{31}P{^{1}H} NMR (162 MHz, benzene-d_6, ppm): δ: 811.42, -635.59. Anal. Calcd for $C_{48}H_{72}N_6P_4U$: C, 52.65; H, 6.63; N, 7.67; Found: C, 52.56; H, 6.78; N, 6.44. Satisfactory elemental analysis could not be obtained despite multiple attempts on crystalline samples from different batches, which probably due to the high sensitivity or incomplete combustion.

Transformation between complex 2 and complex 3.

A suspension of KC_8 (6.8 mg, 0.05 mmol, 2 equiv.) in THF (2 mL) was added to a solution of complex **3** (27.4 mg, 0.025 mmol, 1 equiv.) in THF (2 mL) and stirred for 4 h, during which time the golden color of the KC_8 faded. The solution was filtered, extracted with Et_2O, and then dried *in vacuo* to generate a dark brown powder. NMR characterization of this powder corroborated the formation of **2**. NMR yield: 95%.

A solution of Ph_3CBr (6.5 mg, 0.02 mmol, 2 equiv.) in THF (2 mL) was added to a solution of complex **2** (11.7 mg, 0.01 mmol, 1 equiv.) in THF (2 mL) and stirred for 3

h. The solvent was then removed to yield a brown powder. After extraction of the reaction mixture with toluene, NMR characterization was performed, showing the structure to be consistent with complex **3**. NMR yield: 70%.

2. Supporting Figures

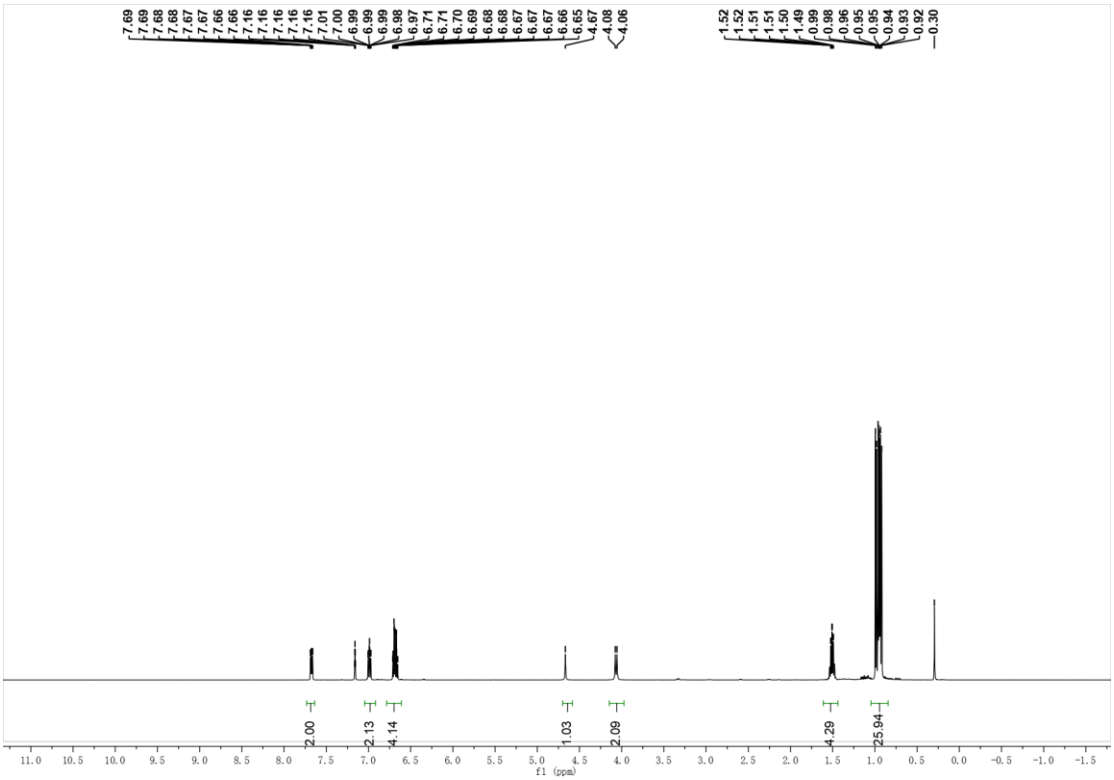

Figure S1. The ^{1}H NMR (400 MHz, 298 K) spectrum of compound **1** in benzene-d_6.

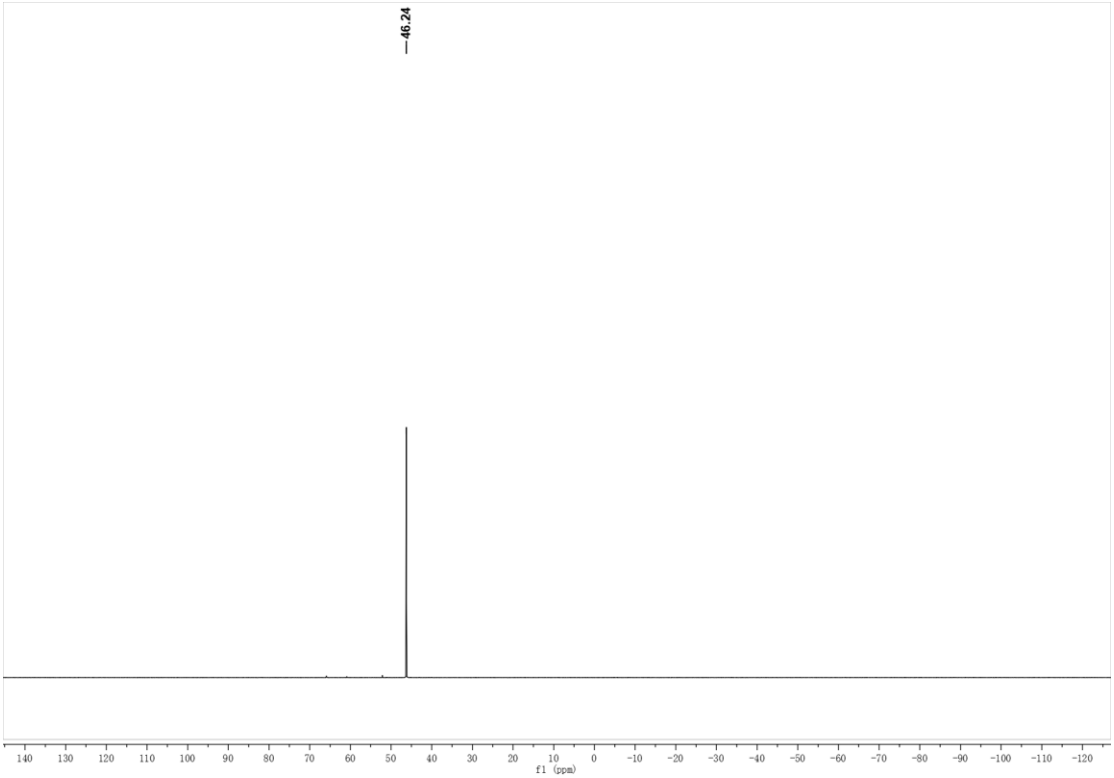

Figure S2. $^{31}P\{^{1}H\}$ NMR (162 MHz, 298 K) spectrum of compound **1** in benzene-d_6.

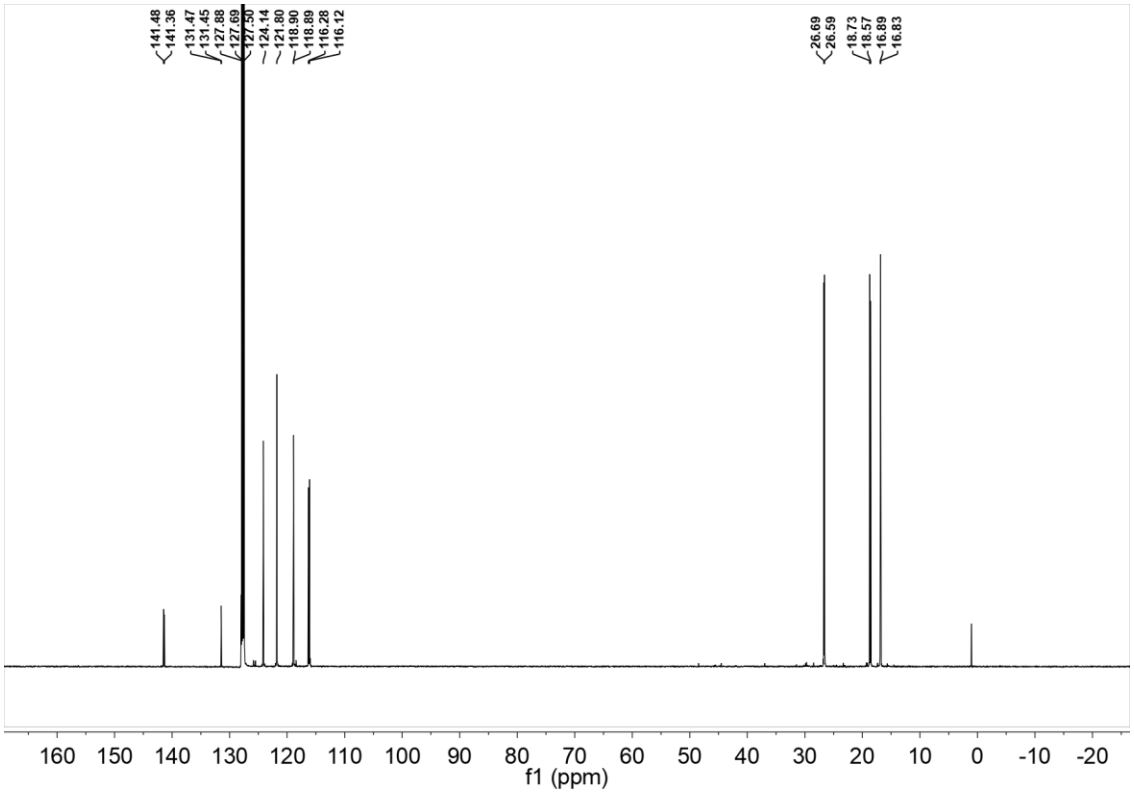

Figure S3. $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K) spectrum of compound **1** in benzene-d_6.

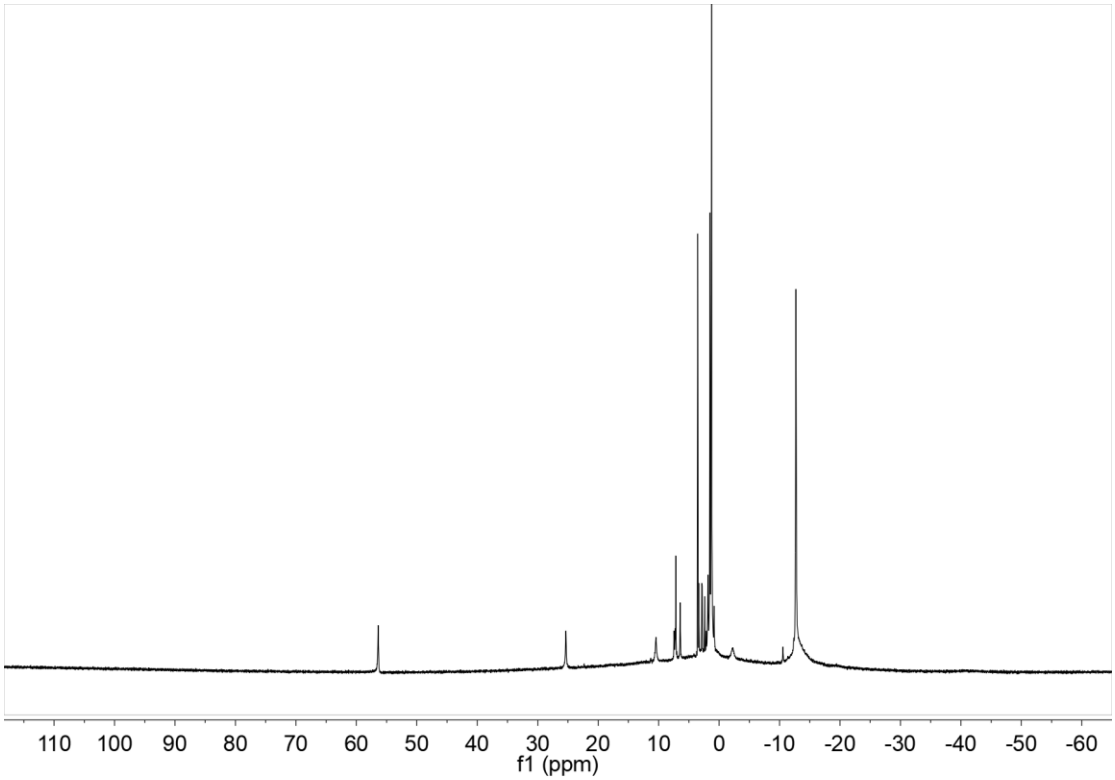

Figure S4. The *in-situ* ^{1}H NMR (400 MHz, 298 K) spectrum of complex **2** in benzene-d_6.

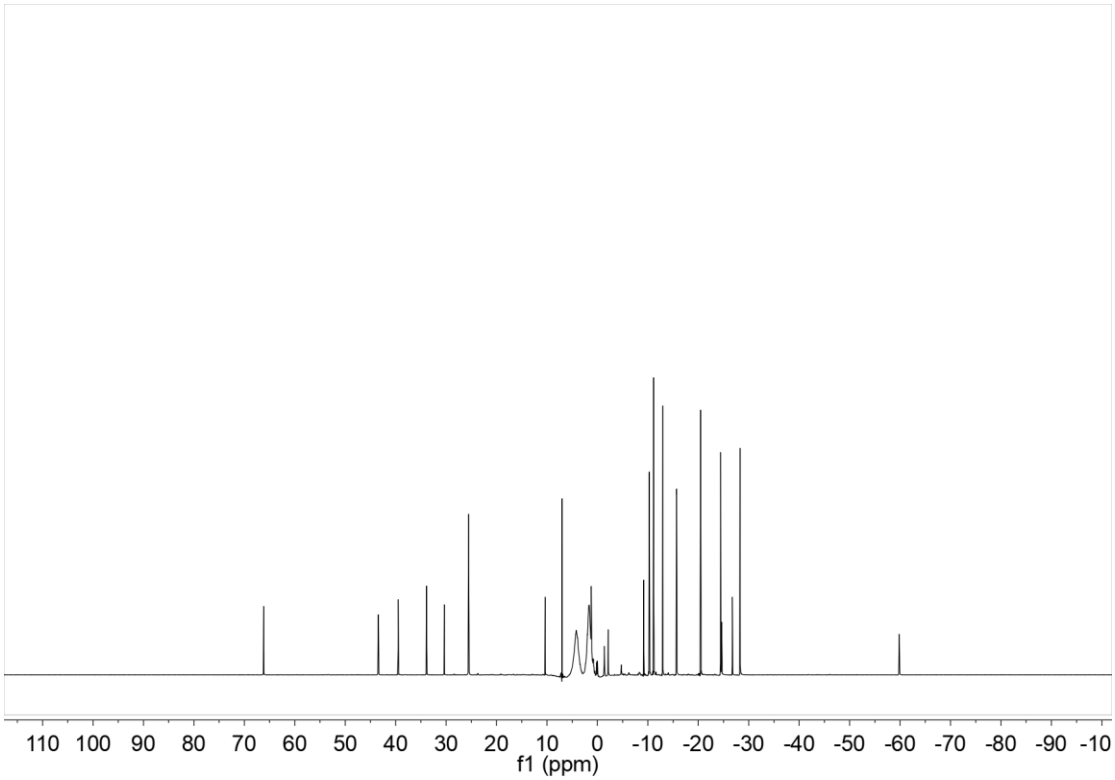

Figure S5. The *in-situ* ^{1}H NMR (400 MHz, 298 K) spectrum of complex **3** in benzene-d_6.

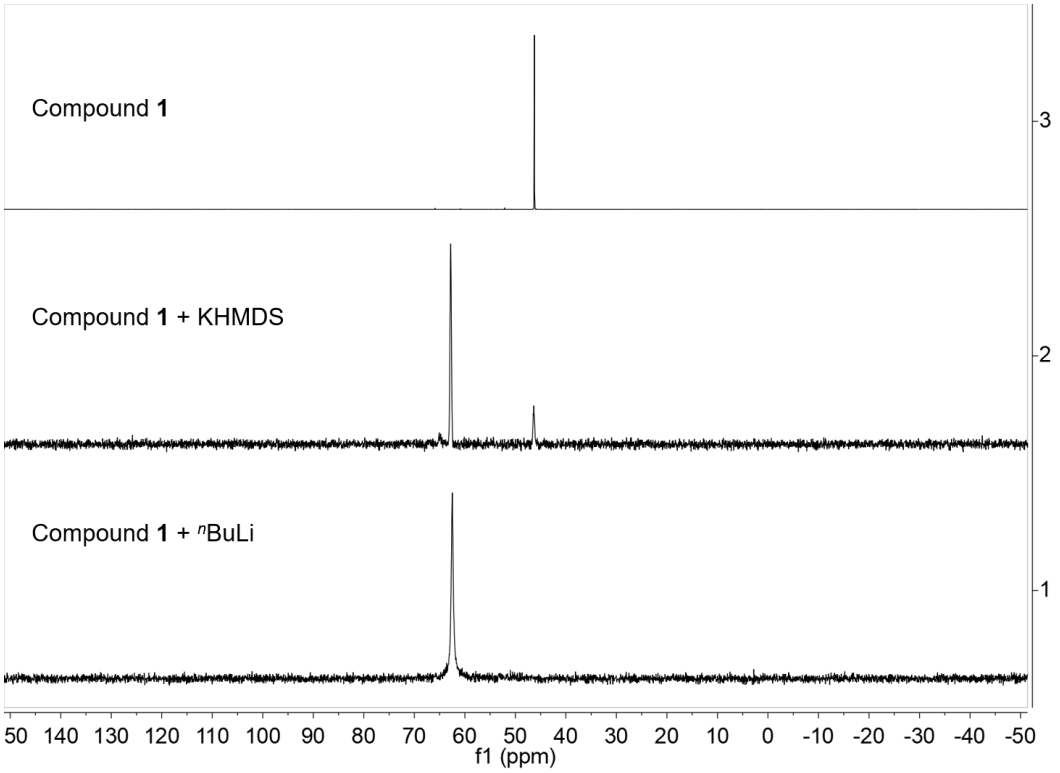

Figure S6. The *in-situ* ^{31}P{^{1}H} NMR (162 MHz, 298 K) spectra for the reactions of compound **1** with ^{n}BuLi and KHMDS in benzene-d_6.

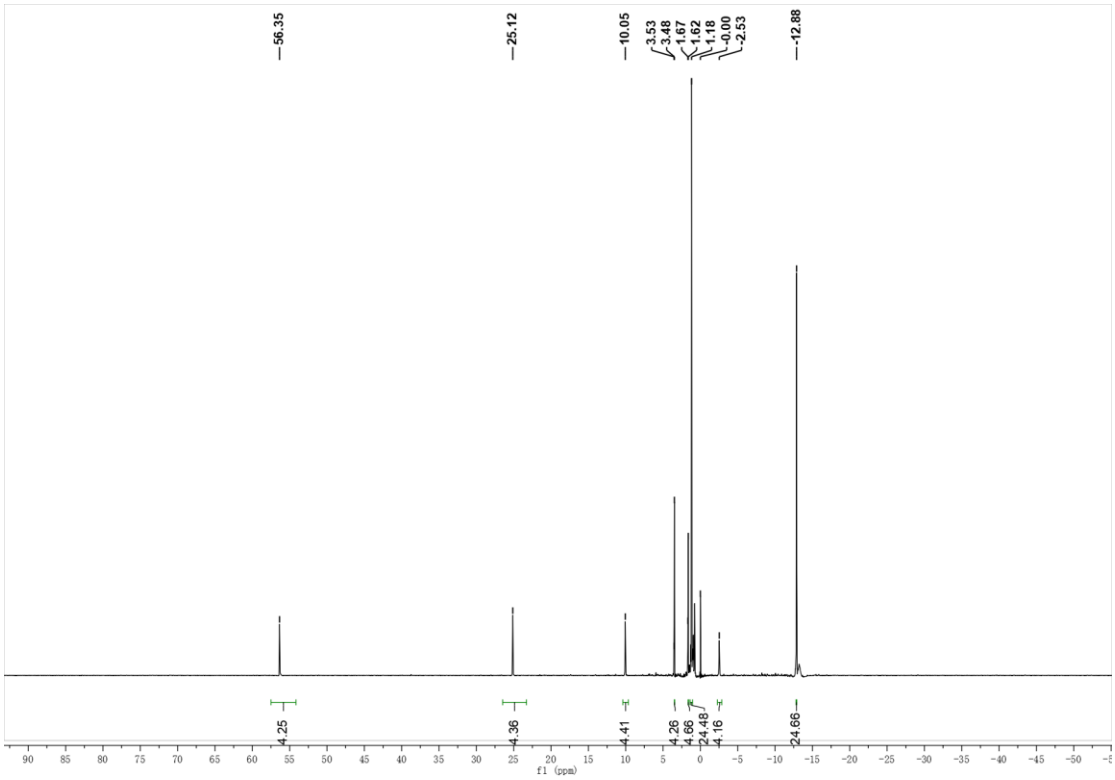

Figure S7. ^{1}H NMR (400 MHz, 298 K) spectrum of complex **2** in tetrahydrofuran-d_8.

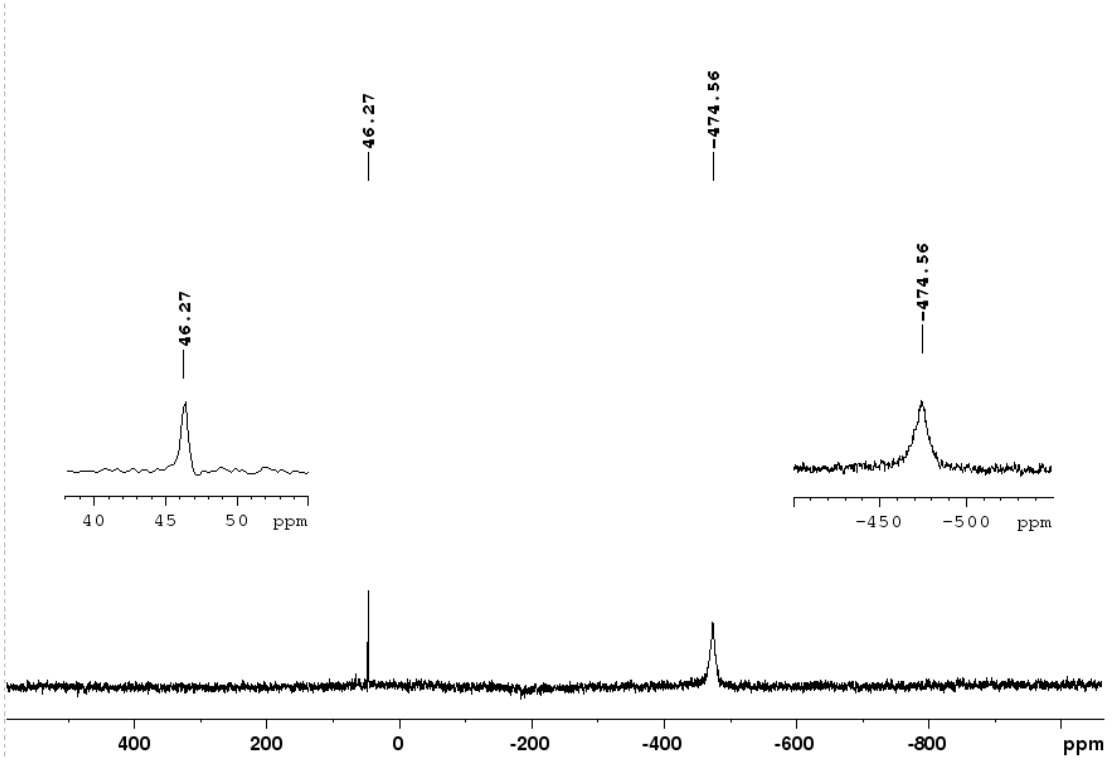

Figure S8. ^{31}P{^{1}H} NMR (162 MHz, 298 K) spectrum of complex **2** in tetrahydrofuran-d_8 (the signal at 46.27 ppm was assigned to compound **1**).

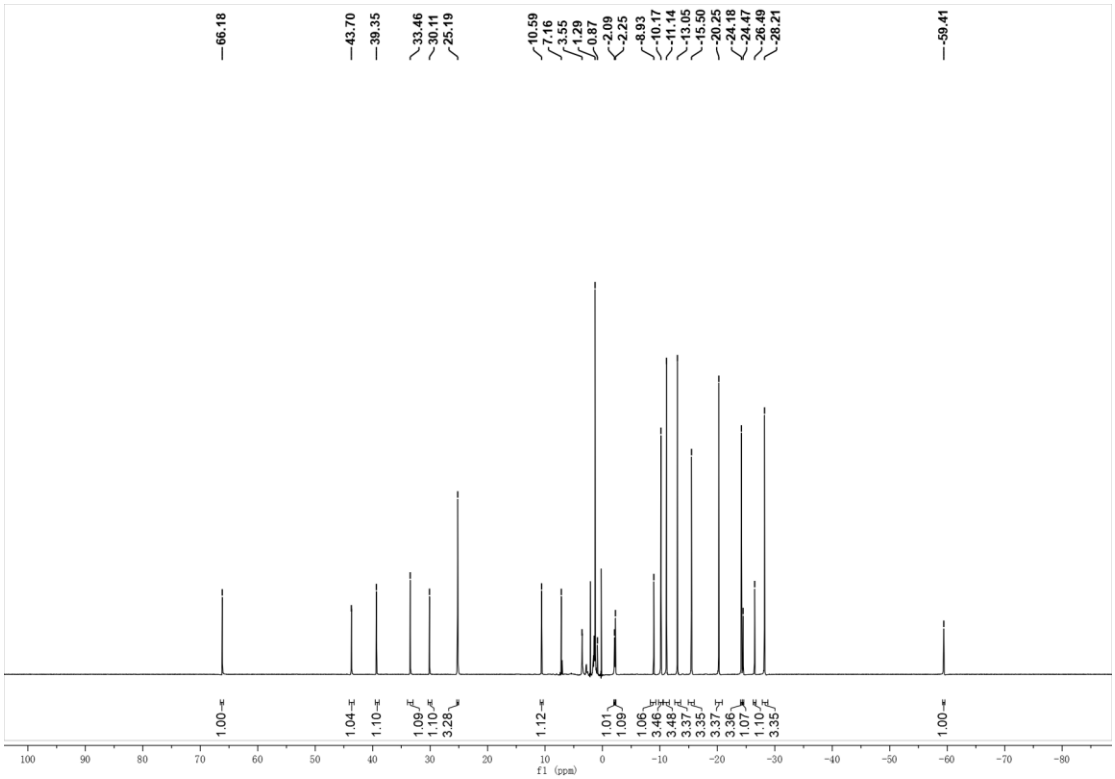

Figure S9. ^{1}H NMR (400 MHz, 298 K) spectrum of complex **3** in benzene-d_6.

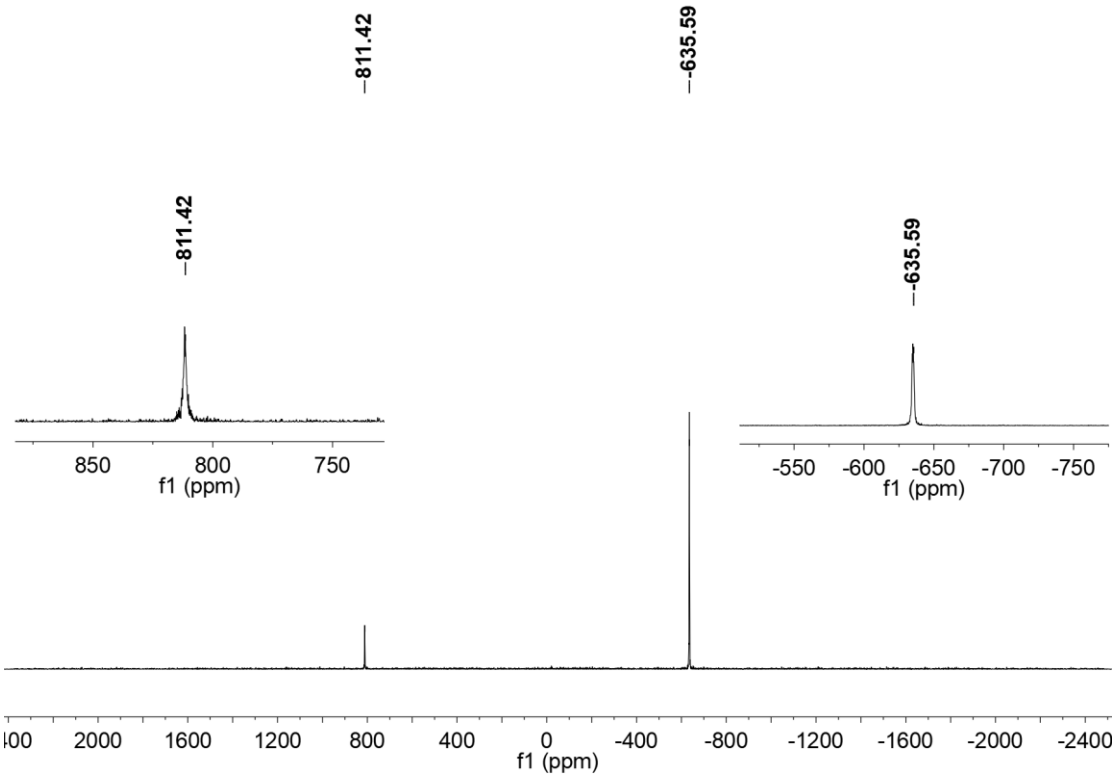

Figure S10. ^{31}P{^{1}H} NMR (162 MHz, 298 K) spectrum of complex **3** in benzene-d_6.

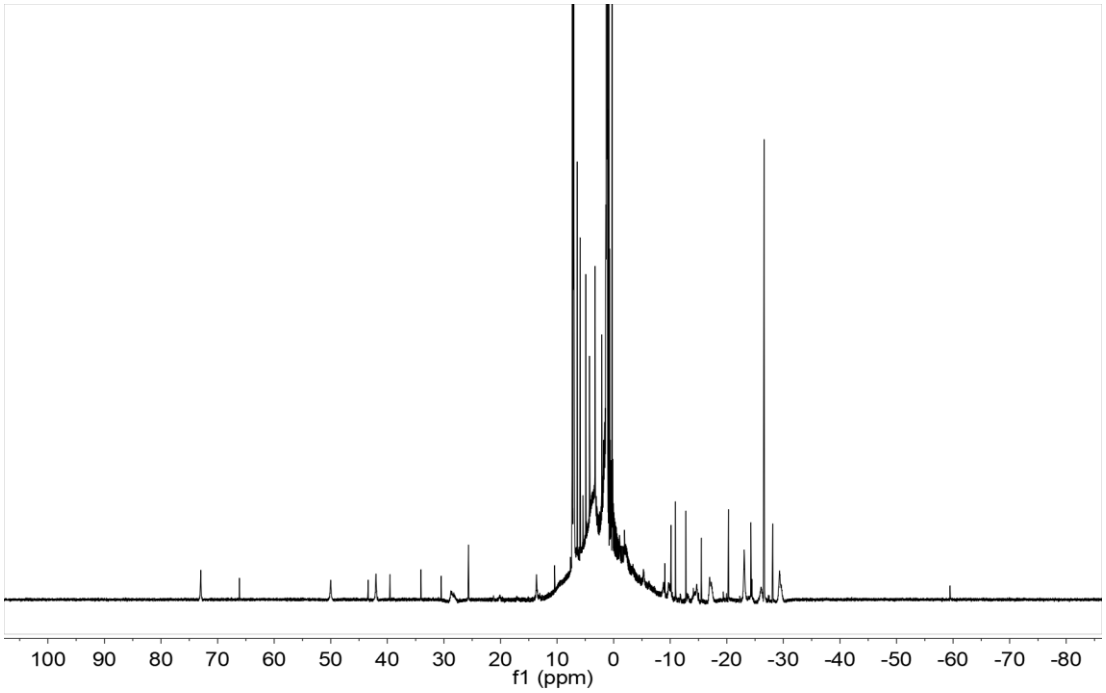

Figure S11. The *in-situ* ^{1}H NMR (400 MHz, 298 K) spectrum for the reaction of Ph_3CBr with complex **2** in benzene-d_6.

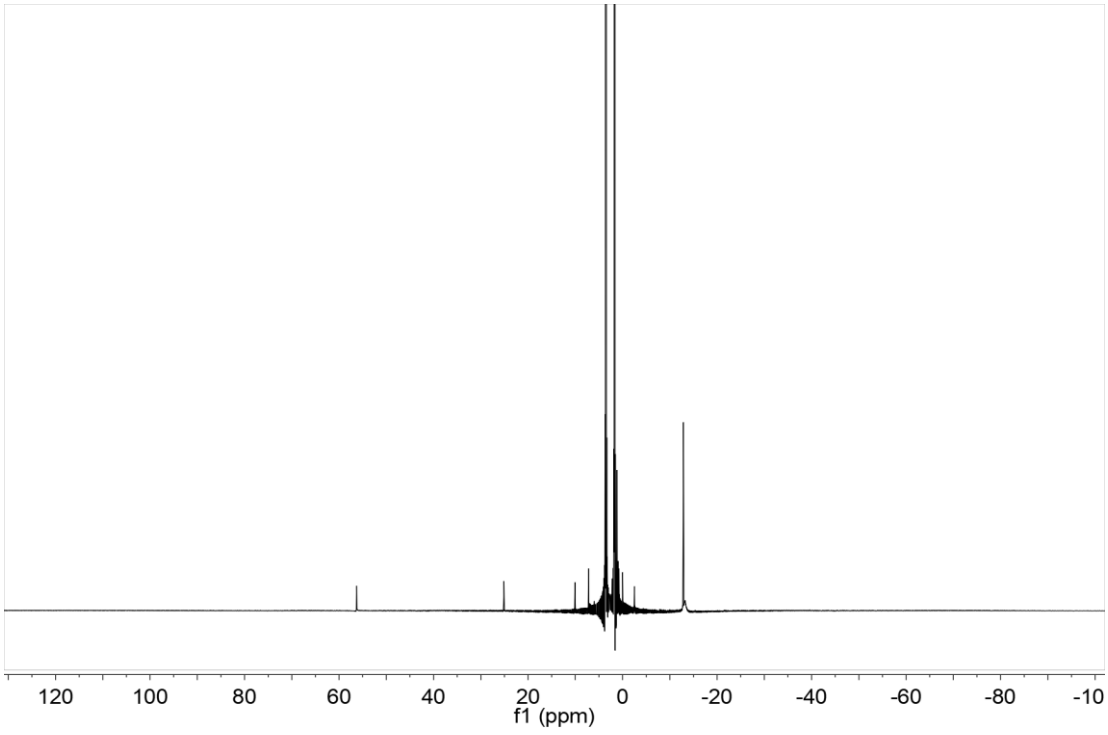

Figure S12. The *in-situ* ^{1}H NMR (400 MHz, 298 K) spectrum for the reaction of KC_8 with complex **3** in tetrahydrofuran-d_8.

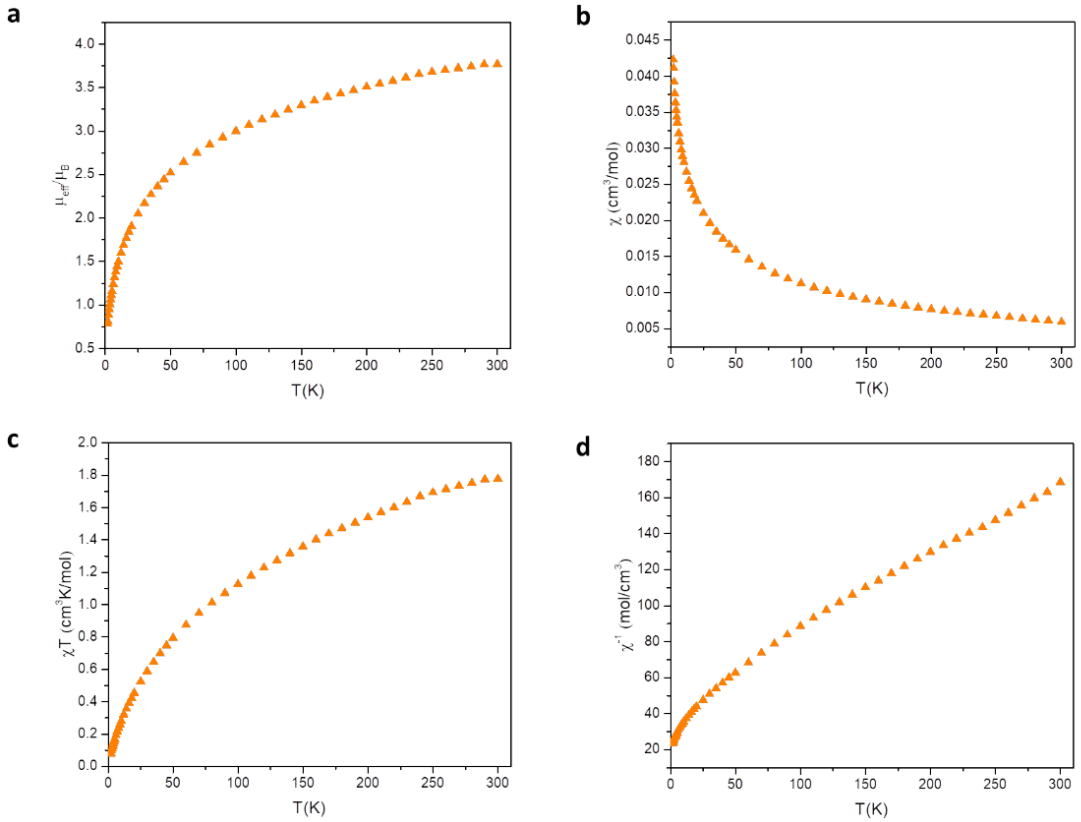

Figure S13. Variable-temperature magnetic data of **2**. (a) μ_{eff} vs T, (b) χ vs T, (c) χT vs T, and (d) 1/χ vs T.

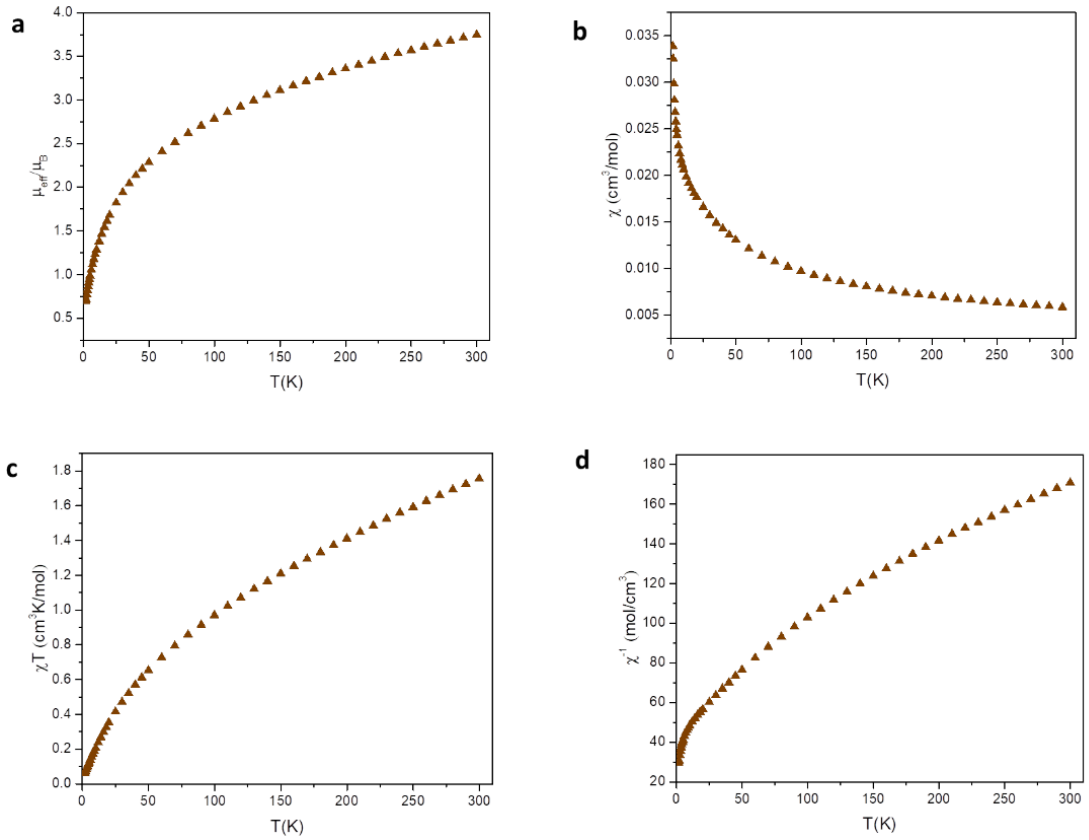

Figure S14. Variable-temperature magnetic data of **3**. (a) μ_{eff} vs T, (b) χ vs T, (c) χT vs T, and (d) 1/χ vs T.

3. X-ray crystallographic analysis

Single-crystal X-ray diffraction data for complexes **2** and **3** were collected on a Bruker D8 venture photon II detector with a radiation source of Ga(Kα) (λ = 1.34139 Å) or Mo(Kα) (0.71073 Å). Multiscan or empirical absorption corrections (SADABS) were applied. These structures were solved using Patterson methods, expanded using difference Fourier syntheses, and refined using full-matrix least squares fitting on F^2 using the Bruker SHELXTL-2014 program package.[3,4] All non-hydrogen atoms were refined on F^2 by full-matrix least-squares procedures with the use of anisotropic displacement parameters. Hydrogen atoms were introduced at their geometric positions and refined as riding atoms. Evaluation of the CIF using the CheckCIF routine at www.checkcif.iucr.org gave no A or B alert for these complexes. Details of the data collection and refinement for complexes **2** and **3** are given in Table S1. CCDC-2102549 (**2**) and 2102548 (**3**) contain the crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data-request/cif.

Table S1. Crystal data and structural refinements for complexes **2** and **3**.

	2-Et_2O	**3**
empirical formula	$C_{146}H_{222}K_6N_{18}OP_{12}U_3$	$C_{48}H_{72}N_6P_4U$
formula weight	3552.67	1095.02
temperature, K	192.99	296.15
wavelength, Å	1.34139	0.71073
crystal system	Monoclinic	Monoclinic
space group	$C2/_C$	$P2_1/c$
a, Å	32.9263(10)	22.2995(9)

b, Å	26.2249(9)	18.4153(8)
c, Å	25.9999(14)	26.0924(10)
α, °	90	90
β, °	121.2940(10)	112.9960(10)
γ, °	90	90
V, Å^3	19184.4(14)	9863.4(7)
Z	4	8
ρ_{calcd}, g cm^{-3}	1.230	1.475
μ, mm^{-1}	6.591	3.460
F(000)	7188.0	4432.0
crystal size, mm	0.12 × 0.10 × 0.10	0.12 × 0.10 × 0.10
θ_{max},°	53.939	27.508
reflns collected	125416	71494
indep reflns	17602 [R_{int} = 0.0739, R_{sigma} = 0.0418]	22594 [R_{int} = 0.1085, R_{sigma} = 0.1197]
data/restraints/params	17602/324/983	22594/13/1106
goodness-of-fit on F^2	1.065	1.047
final *R* ($I > 2\sigma(I)$)	R_1 = 0.0393, wR_2 = 0.1138	R_1 = 0.0687, wR_2 = 0.1080
R indices (all data)	R_1 = 0.0452, wR_2 = 0.1171	R_1 = 0.1365, wR_2 = 0.1356
Residual electron density (e. Å^{-3}) max/min	2.27/-1.26	1.04/-1.35

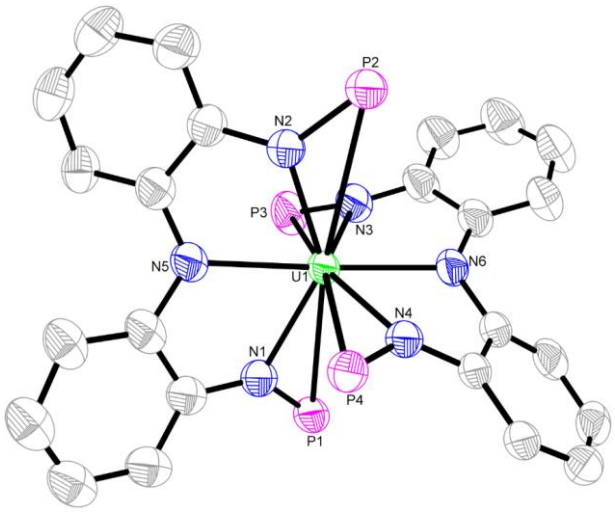

Figure S15. Crystal structure of complex **2**. Thermal ellipsoids are drawn at 50% probability. Hydrogen atoms, isopropyl moieties in P^iPr_2 and potassium cations are omitted for clarity.

Table S2. Selected bond lengths (Å) and angles [°] for complex **2**

U1-P1	3.2010(15)	U1-N4	2.416(4)
U1-P2	3.4504(18)	U1-N5	2.397(5)
U1-P3	3.1579(17)	U1-N6	2.384(4)
U1-P4	3.3894(14)	P1-N1	1.664(6)
U1-N1	2.357(4)	P2-N2	1.686(5)
U1-N2	2.426(5)	P3-N3	1.672(5)
U1-N3	2.321(5)	P4-N4	1.677(5)
P1-U1-P2	171.72(4)	N3-U1-N2	91.66(19)
P1-U1-P4	90.41(4)	N3-U1-N4	131.92(16)
P3-U1-P1	83.13(5)	N3-U1-N5	115.91(16)
P3-U1-P2	102.10(5)	N3-U1-N6	65.89(16)

P3-U1-P4	170.86(4)	N4-U1-P1	85.95(10)
P4-U1-P2	85.08(5)	N4-U1-P2	86.84(10)
N1-U1-P1	30.27(13)	N4-U1-P3	156.55(12)
N1-U1-P2	153.32(14)	N4-U1-P4	27.61(11)
N1-U1-P3	92.93(12)	N4-U1-N2	100.77(16)
N1-U1-P4	78.31(12)	N5-U1-P1	94.60(11)
N1-U1-N2	130.49(17)	N5-U1-P2	91.83(11)
N1-U1-N4	87.91(14)	N5-U1-P3	90.07(11)
N1-U1-N5	65.96(16)	N5-U1-P4	83.99(10)
N1-U1-N6	117.43(16)	N5-U1-N2	65.53(15)
N2-U1-P1	160.13(11)	N5-U1-N4	111.49(15)
N2-U1-P2	26.76(11)	N6-U1-P1	89.34(11)
N2-U1-P3	96.45(13)	N6-U1-P2	84.02(11)
N2-U1-P4	87.43(13)	N6-U1-P3	92.89(11)
N3-U1-P1	97.70(14)	N6-U1-P4	93.49(10)
N3-U1-P2	84.12(14)	N6-U1-N2	110.50(15)
N3-U1-P3	31.00(12)	N6-U1-N4	66.24(15)
N3-U1-P4	157.58(12)	N6-U1-N5	175.34(15)
N3-U1-N1	118.14(18)		

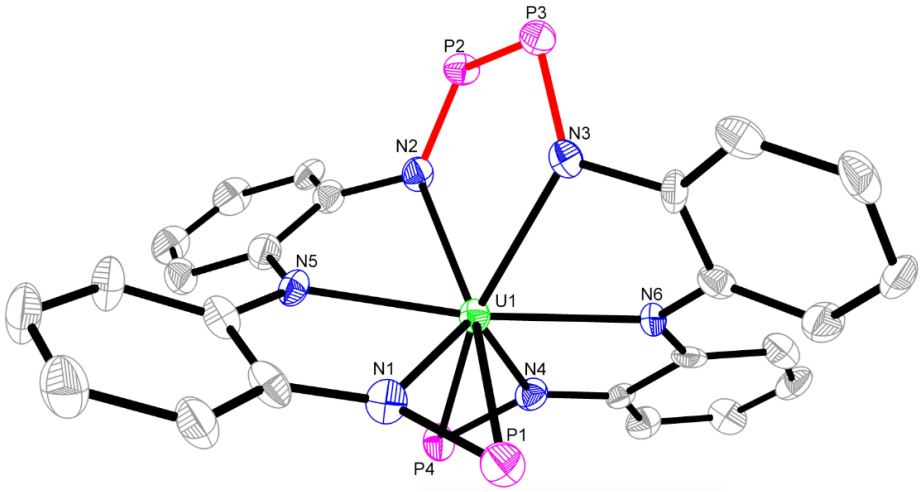

Figure S16. Crystal structure of complex **3**. Thermal ellipsoids are drawn at 50% probability. Hydrogen atoms and isopropyl moieties in P^iPr_2 are omitted for clarity.

Table S3. Selected bond lengths (Å) and angles [°] for complex **3**

U1-P4	3.109(2)	U1-N5	2.398(7)
U1-P1	2.992(2)	P2-P3	2.272(3)
U1-N2	2.497(7)	P2-N2	1.606(7)
U1-N3	2.494(7)	P3-N3	1.593(8)
U1-N6	2.389(7)	P4-N4	1.666(7)
U1-N4	2.308(7)	P1-N1	1.650(7)
U1-N1	2.311(6)		
P1-U1-P4	108.22(7)	N4-U1-N3	124.0(2)
N5-U1-P1	97.70(17)	N1-U1-P1	33.20(18)
N5-U1-P4	88.67(16)	N1-U1-P4	104.91(17)
N5-U1-N2	66.0(2)	N1-U1-N5	64.5(2)
N5-U1-N3	107.5(2)	N1-U1-N2	126.5(2)

N2-U1-P1	153.39(16)	N1-U1-N6	119.7(2)
N2-U1-P4	92.87(16)	N1-U1-N3	102.5(2)
N6-U1-P1	86.64(17)	N3-U1-P1	92.29(16)
N6-U1-P4	95.98(17)	N3-U1-P4	152.17(15)
N6-U1-N5	172.3(2)	N3-U1-N2	74.3(2)
N6-U1-N2	107.6(2)	N2-P2-P3	102.2(3)
N6-U1-N3	65.9(2)	N3-P3-P2	101.0(3)
N4-U1-P1	109.60(19)	N1-P1-U1	50.1(2)
N4-U1-P4	31.65(18)	N4-P4-U1	46.6(2)
N4-U1-N5	119.0(2)	P2-N2-U1	126.3(4)
N4-U1-N2	96.9(2)	P4-N4-U1	101.7(3)
N4-U1-N6	64.8(2)	P1-N1-U1	96.7(3)
N4-U1-N1	124.2(2)	P3-N3-U1	127.8(4)

4. Theoretical Calculations

Computational Details. All calculations were carried out at the DFT level of theory using the hybrid functional B3PW91,[5,6] with the Gaussian 09 suite of programs.[7] The U, and P atoms were represented with a small-core Stuttgart-Dresden relativistic effective core potential associated with their adapted basis set.[8-10] All the other atoms were described with a 6-31G (d,p), double-ζ quality basis set.[11-13] The nature of the extrema (minimum) was established with analytical frequencies calculations and geometry optimisations were computed without any symmetry constraints. The enthalpy energy was computed at T = 298 K. Intrinsic Reaction Coordinates (IRC) were carried out to verify the connections of the optimised transition states.

	H (Hartree)	ΔH (kcal mol^{-1})	G (Hartree)	ΔG (kcal mol^{-1})
2^{ox}	-2702.5	x	-2702.7	x
3	-2702.5	-3.0	-2702.7	x
Int1	-2702.5	2.2	-2702.7	3.0
TS-U-PP	-2702.5	19.5	-2702.7	19.5
IRCB-U-PP	-2702.5	11.7	-2702.7	12.7

	E (u.a.)	H (u.a.)	G (u.a.)
Br^-	-2574.29786782	-2574.295507	-2574.314043
Ph_3CBr	-3306.99954860	-3306.701106	-3306.765060
Ph_3C^-	-732.803710138	-732.511566	-732.569723
Anionic part of 2	-2703.78070393	-2702.601079	-2702.776438

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Anionic part of 2

C	7.668286	14.699633	-0.122773
C	6.417792	14.700938	0.520496
C	5.234921	14.559877	-0.278055
C	5.373616	14.508000	-1.668805
C	6.625723	14.547541	-2.292251
C	7.775682	14.626549	-1.513966
N	4.053711	14.443691	0.453008
P	2.424012	14.833325	0.070335
C	1.610015	13.791885	-1.337093
C	2.138025	13.748204	-2.771076
N	6.205852	14.740591	1.888351
C	7.115619	15.292807	2.775042
C	7.021365	14.827148	4.131464
C	7.932494	15.337498	5.067375
C	8.882071	16.308645	4.731639
C	8.923334	16.806899	3.433834
C	8.043196	16.305852	2.471854
N	6.004216	13.906015	4.380392
P	6.084182	12.578886	5.488921
C	7.921968	12.054264	5.551237
C	8.072661	10.836439	6.466609
P	4.966290	10.549858	2.199342
C	5.157759	9.867804	0.404186
C	4.116506	8.937361	-0.214791
C	5.809440	13.110711	7.325528
C	4.410906	13.710662	7.441139
N	3.592590	11.583449	2.383844
C	2.259454	11.211279	2.536477
C	1.643474	10.068616	2.007911
C	0.276706	9.816039	2.172061
C	-0.510231	10.727767	2.866632
C	0.077857	11.866230	3.424925
C	1.457216	12.114806	3.315964
N	2.126006	13.212888	3.830542

C	1.673307	13.942089	4.917559
C	2.188573	15.280586	5.016428
C	1.803227	16.066744	6.112300
C	0.950120	15.579786	7.109529
C	0.478986	14.274095	7.029202
C	0.843713	13.465823	5.948668
N	3.056960	15.660281	3.993615
P	3.203163	17.263166	3.356653
C	4.062772	18.400130	4.666379
C	4.866203	19.470075	3.918968
C	4.571787	8.925862	3.137231
C	5.820785	8.039288	3.156634
U	4.165473	13.898046	2.798617
C	2.373033	16.629990	-0.614314
C	3.432560	17.130855	-1.595284
C	1.433987	18.004741	3.478576
C	1.404886	19.400248	2.851850
C	4.103723	9.239361	4.557244
C	5.456159	11.048126	-0.518129
C	0.417257	17.080308	2.814740
C	0.965743	16.962105	-1.117851
C	4.982475	17.614353	5.595480
C	6.825882	13.957268	8.090224
C	1.375322	12.377405	-0.806736
C	8.408245	11.742070	4.136007
H	2.195967	17.075307	6.195229
H	2.243624	9.375258	1.432869
H	3.770282	8.384969	2.620240
H	6.092159	9.295590	0.523188
H	-0.540305	12.584934	3.953918
H	1.174056	18.095051	4.540097
H	4.479100	14.441320	-2.273762
H	4.596513	11.720731	-0.588634
H	5.703174	10.708512	-1.533701
H	6.292482	11.650697	-0.151893
H	8.068626	16.701448	1.461149
H	9.632605	17.586647	3.160048
H	0.491790	12.439874	5.904444
H	2.534112	17.174211	0.326696
H	-1.581767	10.566948	2.976499
H	7.878992	14.980342	6.087481
H	3.276719	18.891070	5.260628
H	5.786262	12.112881	7.792922
H	-0.166770	13.869528	7.807328

H	0.630800	14.295160	-1.361525
H	-0.161048	8.918206	1.738462
H	0.675223	16.220986	7.945397
H	4.434370	16.870021	6.177206
H	5.490914	18.293327	6.295870
H	5.757448	17.083499	5.034564
H	8.530601	12.873888	5.951699
H	8.761033	14.629174	-1.977918
H	6.688978	14.503776	-3.378347
H	9.565238	16.680119	5.493701
H	4.819068	9.886433	5.076015
H	3.985286	8.310562	5.135181
H	3.143098	9.760033	4.550258
H	7.855714	13.599614	7.974258
H	6.597628	13.950073	9.167255
H	6.790595	15.002095	7.766232
H	4.354967	14.669836	6.918916
H	4.136240	13.884278	8.490811
H	3.648161	13.065504	6.995758
H	8.567046	14.748704	0.484236
H	5.681500	19.002365	3.355805
H	5.313719	20.188847	4.621046
H	4.258269	20.035276	3.203902
H	0.675853	16.883963	1.770399
H	-0.584962	17.533283	2.838130
H	0.367759	16.113506	3.319961
H	6.136904	7.734877	2.152715
H	5.634438	7.122405	3.734433
H	6.663930	8.559697	3.625878
H	3.872117	8.085488	0.430397
H	4.485595	8.527474	-1.167611
H	3.187545	9.472973	-0.433070
H	2.045559	20.109715	3.386271
H	0.383560	19.808224	2.863605
H	1.736526	19.374912	1.806430
H	2.321130	11.844432	-0.671087
H	0.760884	11.794098	-1.507754
H	0.873046	12.382003	0.164015
H	0.777570	16.521263	-2.104688
H	0.837445	18.049089	-1.219657
H	0.186277	16.599963	-0.438077
H	2.347095	14.742333	-3.178711
H	1.398792	13.269679	-3.432631
H	3.053759	13.153199	-2.837578

H	4.442455	16.956547	-1.222007
H	3.308811	18.213961	-1.752871
H	3.354243	16.650373	-2.576662
H	7.750057	11.019969	3.640648
H	9.426968	11.327532	4.161123
H	8.422437	12.641197	3.515351
H	7.806956	11.057073	7.506598
H	9.110944	10.473969	6.461610
H	7.434615	10.010136	6.130327

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Br-

Br	-0.895665	-1.551343	-0.633338

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Ph3C-

C	0.469555	0.811959	0.332735
C	0.245528	0.510062	1.737782
C	1.711445	0.410485	-0.309672
C	-0.548875	1.516302	-0.431055
C	1.786788	0.078766	-1.691971
C	2.973693	-0.299167	-2.305496
C	4.168131	-0.384886	-1.583014
C	4.128160	-0.070482	-0.220777
C	2.945579	0.319087	0.393934
H	0.874363	0.109778	-2.281149
H	2.962988	-0.550183	-3.366082
H	5.096061	-0.685504	-2.063850
H	5.042144	-0.111651	0.371590
H	2.959725	0.580057	1.448610
C	-0.231840	2.385898	-1.512405
C	-1.205519	3.053139	-2.243773
C	-2.563754	2.910321	-1.942436
C	-2.909583	2.066870	-0.881742
C	-1.939520	1.389145	-0.155261
H	0.814478	2.541376	-1.760893
H	-0.897066	3.712907	-3.054636
H	-3.324937	3.436848	-2.513407
H	-3.959008	1.919525	-0.626931
H	-2.248498	0.723221	0.645843
C	-0.547518	1.336567	2.583083
C	-0.763968	1.044323	3.923141
C	-0.196492	-0.086280	4.519772
C	0.592205	-0.917686	3.718122

C	0.801678	-0.635166	2.374885
H	-0.985390	2.237392	2.161749
H	-1.373686	1.723018	4.519441
H	-0.363211	-0.311310	5.570579
H	1.038688	-1.816069	4.144197
H	1.399557	-1.319235	1.778878

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Ph3CBr

C	0.074098	0.041405	0.098172
C	0.020129	0.113656	1.622089
C	1.500076	-0.040209	-0.440017
C	-0.746173	1.141171	-0.570822
C	1.734713	-0.388749	-1.779399
C	3.024558	-0.409622	-2.295964
C	4.112323	-0.075359	-1.486876
C	3.891461	0.285606	-0.162234
C	2.595678	0.305291	0.357913
H	0.895118	-0.655648	-2.413824
H	3.181803	-0.691422	-3.333426
H	5.121300	-0.097199	-1.889219
H	4.727015	0.553714	0.478500
H	2.441807	0.596146	1.391119
C	-0.123010	2.187938	-1.258660
C	-0.874995	3.228646	-1.807269
C	-2.259339	3.241918	-1.675004
C	-2.890518	2.208452	-0.980109
C	-2.142410	1.173407	-0.432024
H	0.956123	2.198315	-1.365083
H	-0.368477	4.028587	-2.340308
H	-2.844603	4.048457	-2.107835
H	-3.971093	2.206693	-0.866940
H	-2.641677	0.371439	0.102824
C	-0.381679	1.284733	2.273331
C	-0.366456	1.367544	3.667018
C	0.053100	0.284219	4.431492
C	0.467601	-0.885375	3.791603
C	0.454239	-0.967843	2.404286
H	-0.705501	2.141829	1.693387
H	-0.687289	2.286529	4.149822
H	0.058281	0.346531	5.516146
H	0.799482	-1.739302	4.375680
H	0.772859	-1.883362	1.915618
Br	-0.822307	-1.730051	-0.417537

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2^{ox}

C	7.560677	14.682912	-0.306288
C	6.341403	14.698390	0.402103
C	5.109834	14.555529	-0.313890
C	5.156849	14.459435	-1.713429
C	6.366925	14.480723	-2.394122
C	7.573234	14.576820	-1.689058
N	3.986869	14.481921	0.483064
P	2.297933	14.743882	0.168024
C	1.582620	13.655543	-1.243434
C	1.613626	14.083640	-2.712233
N	6.196336	14.745059	1.769999
C	7.127194	15.298159	2.616508
C	6.991590	14.910936	3.992140
C	7.924641	15.413126	4.916922
C	8.925087	16.294288	4.526336
C	9.009350	16.724948	3.196627
C	8.116887	16.237262	2.254824
N	5.924414	14.073864	4.259364
P	5.905449	12.723056	5.382598
C	7.720007	12.141061	5.468338
C	7.845601	10.951635	6.425961
P	5.025276	10.744871	2.310455
C	5.430524	10.021575	0.588590
C	4.434892	9.104329	-0.117418
C	5.614102	13.232729	7.202206
C	4.161108	13.664145	7.390248
N	3.548027	11.693872	2.331550
C	2.262579	11.226823	2.484029
C	1.729752	10.049372	1.926546
C	0.390593	9.718005	2.085638
C	-0.475669	10.561982	2.795786
C	0.017699	11.711017	3.386927
C	1.389555	12.044049	3.287635
N	1.988626	13.146642	3.825444
C	1.490599	13.870254	4.867257
C	2.039215	15.199760	4.977855
C	1.561183	16.029274	6.013258
C	0.638117	15.562466	6.937149
C	0.163409	14.242124	6.872187
C	0.581944	13.409393	5.850942
N	2.982441	15.525175	4.041476

P	3.413233	17.117971	3.454795
C	4.367552	18.116801	4.796577
C	5.523733	18.848110	4.106132
C	4.626124	9.142966	3.271338
C	5.880965	8.266449	3.348987
U	4.149766	13.932090	2.743520
C	2.131075	16.545024	-0.425516
C	3.050792	17.061930	-1.532336
C	1.798957	18.149505	3.458799
C	2.057824	19.420788	2.643102
C	4.079929	9.426317	4.670058
C	5.908506	11.140352	-0.331398
C	0.581828	17.382971	2.953444
C	0.656931	16.851054	-0.722649
C	4.871117	17.270731	5.960842
C	6.574692	14.175530	7.922826
C	2.101396	12.227027	-1.090799
C	8.254689	11.780374	4.082921
H	1.944864	17.039508	6.099917
H	2.370695	9.418567	1.324918
H	3.860860	8.594914	2.709496
H	6.313326	9.421526	0.857301
H	-0.656709	12.393216	3.892886
H	1.610750	18.449734	4.496865
H	4.227131	14.356745	-2.257454
H	5.097439	11.832708	-0.569647
H	6.282522	10.731343	-1.277866
H	6.714033	11.724309	0.123119
H	8.153686	16.599671	1.233184
H	9.761044	17.452438	2.902899
H	0.256014	12.375241	5.826265
H	2.410337	17.075801	0.493968
H	-1.534327	10.328309	2.864601
H	7.836731	15.130982	5.957925
H	3.659952	18.864752	5.180936
H	5.714370	12.236306	7.660955
H	-0.515427	13.867903	7.633154
H	0.527638	13.661059	-0.929716
H	0.006715	8.813095	1.621571
H	0.302787	16.219337	7.735638
H	4.053885	16.875043	6.568089
H	5.509843	17.879129	6.614117
H	5.465629	16.425560	5.606182
H	8.321673	12.968319	5.861275

H	8.520703	14.551545	-2.220145
H	6.374203	14.400783	-3.478094
H	9.624409	16.672709	5.267363
H	4.785330	10.016265	5.261178
H	3.896329	8.478135	5.191465
H	3.136363	9.976031	4.641551
H	7.623957	13.880133	7.815277
H	6.353084	14.185177	8.998337
H	6.465867	15.204374	7.565855
H	3.969843	14.634848	6.926358
H	3.921278	13.755693	8.456912
H	3.464297	12.944221	6.950332
H	8.494878	14.710898	0.244646
H	6.271877	18.139215	3.737005
H	6.021576	19.525409	4.811533
H	5.188444	19.445469	3.251366
H	0.775874	16.894446	1.997275
H	-0.262028	18.071016	2.815019
H	0.269933	16.609595	3.658313
H	6.234199	7.938873	2.366565
H	5.665253	7.363399	3.933337
H	6.706663	8.787137	3.846676
H	4.099789	8.273970	0.513782
H	4.899444	8.661750	-1.008532
H	3.555143	9.658855	-0.458571
H	2.901773	20.000219	3.032130
H	1.175193	20.071764	2.668921
H	2.270734	19.189413	1.593710
H	3.149822	12.159555	-1.398964
H	1.523579	11.545308	-1.727362
H	2.027331	11.869724	-0.060873
H	0.346614	16.455287	-1.694242
H	0.494479	17.935127	-0.750238
H	-0.020366	16.436650	0.032215
H	1.231919	15.092872	-2.876764
H	0.981300	13.399319	-3.293491
H	2.614564	14.028335	-3.149362
H	4.104007	16.932047	-1.277693
H	2.875291	18.136507	-1.678986
H	2.872546	16.571326	-2.493494
H	7.711850	10.932905	3.655484
H	9.315532	11.508634	4.153851
H	8.165989	12.610692	3.378234
H	7.632760	11.218321	7.465523

H	8.868653	10.556572	6.395886
H	7.172482	10.133303	6.144283

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Int1

C	3.218263	1.626266	-2.957751
C	2.033121	1.318716	-2.276381
C	0.839767	1.096665	-3.016228
C	0.859060	1.243412	-4.406432
C	2.037945	1.591560	-5.066947
C	3.216300	1.769776	-4.344951
N	-0.223648	0.665014	-2.222640
P	-1.928989	0.509529	-2.494288
C	-2.272656	-0.505293	-4.079206
C	-1.218623	-1.571648	-4.360119
N	1.890407	1.092078	-0.908318
C	2.780289	1.580775	0.043694
C	2.781478	0.869102	1.278876
C	3.650434	1.279369	2.295277
C	4.486342	2.379036	2.124391
C	4.441542	3.111490	0.936864
C	3.588074	2.722635	-0.091175
N	1.845433	-0.163419	1.348202
P	1.715991	-1.582727	2.344481
C	3.294512	-2.611471	2.044772
C	4.659380	-1.922368	2.041300
P	0.586101	-3.744748	-1.479294
C	2.248801	-2.863625	-1.700329
C	3.420829	-3.848522	-1.719991
C	1.697986	-1.257381	4.234918
C	0.597524	-0.257088	4.574437
N	-0.389656	-2.446664	-0.709415
C	-1.711734	-2.743935	-0.577898
C	-2.396042	-3.794279	-1.263208
C	-3.729358	-4.054490	-1.046593
C	-4.478045	-3.275433	-0.134863
C	-3.872148	-2.249325	0.551524
C	-2.496286	-1.956009	0.364645
N	-1.838634	-0.948635	0.976625
C	-2.238756	-0.296805	2.133878
C	-1.773155	1.050164	2.249200
C	-2.078395	1.748716	3.430315
C	-2.813738	1.153927	4.450999
C	-3.245636	-0.170107	4.337087
C	-2.947542	-0.894968	3.189600

N	-1.048219	1.543860	1.165797
P	-1.158572	3.215123	0.580318
C	-0.233523	4.352426	1.824575
C	0.333853	5.540837	1.038661
C	0.936508	-4.920963	0.000721
C	-0.192807	-5.007975	1.022278
U	0.067381	-0.039343	-0.089585
C	-2.585162	2.239225	-2.944472
C	-1.907344	3.000283	-4.082048
C	-2.944682	3.736221	1.035124
C	-3.190336	5.177525	0.578945
C	1.256469	-6.302063	-0.580502
C	2.216911	-2.090509	-3.018727
C	-3.996837	2.797816	0.450772
C	-4.099879	2.182357	-3.168476
C	0.881982	3.653107	2.592529
C	2.963484	-0.956790	5.041848
C	-3.653252	-1.160624	-3.942706
C	3.271753	-3.850424	2.947577
H	-1.714166	2.761922	3.554634
H	-1.842135	-4.375444	-1.993686
H	1.820854	-4.527859	0.512614
H	2.383256	-2.164013	-0.862697
H	-4.450494	-1.613672	1.212864
H	-3.026220	3.704523	2.126742
H	-0.050443	1.082941	-4.973835
H	3.136969	-1.511898	-3.152578
H	1.382309	-1.390572	-3.070693
H	2.121879	-2.781225	-3.864161
H	3.533898	3.307439	-1.002733
H	5.066612	3.991161	0.811269
H	-3.233261	-1.939045	3.111444
H	-2.381385	2.783102	-2.013868
H	-5.539066	-3.465746	-0.001427
H	3.667086	0.724147	3.223220
H	-0.984304	4.724159	2.536662
H	1.348637	-2.254145	4.546091
H	-3.792124	-0.641916	5.148372
H	-2.296175	0.205675	-4.915918
H	-4.217808	-4.847721	-1.605938
H	-3.031040	1.721372	5.351836
H	0.524993	2.787509	3.154740
H	1.342485	4.352792	3.301320
H	1.670888	3.309416	1.919640

H	3.115968	-2.955268	1.019479
H	4.141554	2.015230	-4.858785
H	2.032628	1.709587	-6.146875
H	5.158167	2.673416	2.925794
H	0.376411	-6.727864	-1.075146
H	1.557780	-6.991633	0.217722
H	2.064888	-6.275660	-1.316983
H	3.810721	-1.593620	4.781720
H	2.751180	-1.116248	6.107045
H	3.275575	0.086611	4.943491
H	0.855154	0.743869	4.215743
H	0.463998	-0.195992	5.661190
H	-0.363217	-0.535512	4.137103
H	4.145113	1.732550	-2.404678
H	1.115725	5.204318	0.349442
H	0.782171	6.273102	1.721800
H	-0.423881	6.061149	0.444888
H	-4.077688	2.921512	-0.631138
H	-4.980531	3.027892	0.878430
H	-3.779519	1.746513	0.654417
H	-0.385327	-4.040360	1.490592
H	0.087059	-5.716841	1.812207
H	-1.123965	-5.370447	0.575849
H	3.552327	-4.391651	-0.780497
H	4.351102	-3.304151	-1.918139
H	3.301346	-4.585152	-2.523362
H	-2.553198	5.897905	1.099753
H	-4.230986	5.460895	0.779919
H	-3.020761	5.294044	-0.498026
H	-3.650603	-1.898034	-3.133733
H	-3.911052	-1.683528	-4.872195
H	-4.451455	-0.443863	-3.736520
H	-4.340794	1.757231	-4.148846
H	-4.520060	3.195341	-3.150529
H	-4.619895	1.592269	-2.406926
H	-0.235375	-1.143833	-4.561543
H	-1.513997	-2.159435	-5.238391
H	-1.119971	-2.267730	-3.522180
H	-0.846831	3.168987	-3.891265
H	-2.387018	3.981111	-4.199071
H	-2.007366	2.482087	-5.042859
H	3.502020	-3.604164	3.988613
H	4.025185	-4.573942	2.613848
H	2.298469	-4.352893	2.931378

H	4.689618	-1.085596	1.340947
H	5.429000	-2.643571	1.735311
H	4.945672	-1.542902	3.025492

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C	7.114205	15.495074	-0.518647
C	5.977764	15.012707	0.137014
C	4.794067	14.752713	-0.605437
C	4.771677	15.024285	-1.974033
C	5.906101	15.534339	-2.613475
C	7.073140	15.759301	-1.890750
N	3.787735	14.190765	0.178017
P	2.241164	13.520792	-0.196160
C	2.400929	12.454683	-1.762502
C	3.639549	11.566820	-1.704052
N	5.864150	14.635314	1.471660
C	6.693564	15.073413	2.493246
C	6.736607	14.232386	3.649132
C	7.514356	14.644062	4.742212
C	8.265081	15.813234	4.705258
C	8.205147	16.641283	3.580738
C	7.406794	16.288263	2.501026
N	5.958136	13.062473	3.597165
P	6.399413	11.532125	4.292557
C	8.266829	11.169411	4.047648
C	9.378938	12.090453	4.557080
P	4.952510	9.945734	2.185267
C	6.485451	9.917276	1.106446
C	6.340629	8.901841	-0.033697
C	6.025653	11.503908	6.182694
C	4.750961	12.311568	6.427868
N	3.864913	11.216546	2.075997
C	2.507268	10.796154	2.051907
C	2.024910	9.699451	1.328049
C	0.673179	9.359008	1.354067
C	-0.217467	10.147544	2.084291
C	0.240582	11.252882	2.794080
C	1.607122	11.586735	2.815762
N	2.170743	12.679631	3.453576
C	1.598609	13.284402	4.570176
C	2.044142	14.615942	4.794021
C	1.548580	15.320702	5.896187
C	0.651889	14.723012	6.785061
C	0.256094	13.403278	6.590704

C	0.733151	12.684038	5.494000
N	2.988939	15.058810	3.860627
P	3.392454	16.716363	3.463526
C	4.086964	17.567663	5.039929
C	5.056528	18.675253	4.614374
C	4.763382	8.562982	3.457553
C	3.634698	8.885327	4.433926
U	4.024323	13.638939	2.391044
C	1.073683	14.935797	-0.724531
C	1.051462	15.361282	-2.192058
C	1.704232	17.601941	3.378876
C	1.890247	19.095505	3.101740
C	4.591961	7.184054	2.818585
C	6.812447	11.308076	0.566397
C	0.812039	16.963161	2.323916
C	-0.343004	14.628868	-0.222643
C	4.768743	16.595661	5.996045
C	7.103106	11.845398	7.213035
C	1.120805	11.631034	-1.927676
C	8.509661	9.730308	4.527319
H	1.879703	16.336674	6.078252
H	2.723684	9.119122	0.729339
H	5.717317	8.600604	3.997620
H	7.280236	9.584414	1.786328
H	-0.463000	11.878347	3.332504
H	1.226434	17.480502	4.357158
H	3.873410	14.825442	-2.547114
H	7.744773	11.260798	-0.007457
H	6.923613	12.056639	1.353388
H	6.027488	11.658057	-0.108038
H	7.320044	16.951056	1.647534
H	8.767280	17.570728	3.553715
H	0.440924	11.647672	5.360076
H	1.475659	15.763076	-0.130891
H	-1.277920	9.909723	2.091461
H	7.538555	14.014105	5.623022
H	3.227079	18.027509	5.547368
H	5.782780	10.439848	6.315258
H	-0.421150	12.923660	7.292336
H	2.496359	13.128808	-2.621074
H	0.319017	8.499979	0.791212
H	0.280331	15.290124	7.634096
H	4.092851	15.808900	6.337790
H	5.134375	17.136768	6.878328

H	5.631423	16.121880	5.521546
H	8.331915	11.171562	2.952074
H	7.962189	16.135886	-2.389149
H	5.871908	15.743416	-3.679161
H	8.877702	16.088457	5.559222
H	3.665033	7.125810	2.241629
H	4.544642	6.425452	3.609281
H	5.425762	6.918880	2.162856
H	8.008745	11.245141	7.098286
H	6.709645	11.648785	8.218853
H	7.387824	12.900986	7.189190
H	4.935259	13.383143	6.308665
H	4.386591	12.142088	7.447583
H	3.944985	12.045932	5.737327
H	8.037475	15.640092	0.032314
H	5.932950	18.246668	4.119164
H	5.404883	19.233577	5.492631
H	4.603836	19.393813	3.924632
H	1.200796	17.164991	1.320569
H	-0.200740	17.381031	2.374989
H	0.736005	15.880430	2.455780
H	3.730381	9.889441	4.853119
H	3.664363	8.164968	5.259440
H	2.657866	8.810980	3.951253
H	6.131695	7.890737	0.323687
H	7.274773	8.867595	-0.607729
H	5.538106	9.193866	-0.716830
H	2.387962	19.617562	3.923529
H	0.913549	19.574017	2.958186
H	2.475321	19.262646	2.189578
H	0.956560	10.977750	-1.064727
H	1.191318	11.001207	-2.823345
H	0.233885	12.261450	-2.043169
H	-0.815430	13.832760	-0.808730
H	-0.979357	15.517605	-0.312240
H	-0.346175	14.310826	0.823423
H	4.554587	12.164682	-1.710152
H	3.665221	10.901599	-2.576434
H	3.635235	10.944956	-0.803407
H	2.025082	15.713520	-2.539473
H	0.342565	16.188759	-2.324238
H	0.719571	14.552434	-2.851982
H	8.431779	9.642936	5.615992
H	9.520843	9.408667	4.251171

H	7.807575	9.013909	4.088671
H	9.328409	13.083256	4.111565
H	10.349566	11.651644	4.289409
H	9.365504	12.206291	5.643242

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C	3.136104	1.558366	-3.124528
C	1.943718	1.271252	-2.451215
C	0.759286	1.015471	-3.192954
C	0.799006	1.081035	-4.587632
C	1.991237	1.390572	-5.248602
C	3.154706	1.621630	-4.519885
N	-0.314704	0.671836	-2.373589
P	-2.019735	0.629409	-2.607566
C	-2.448496	-0.481883	-4.099144
C	-1.441425	-1.614599	-4.277430
N	1.770232	1.091170	-1.082887
C	2.624435	1.598036	-0.114514
C	2.658900	0.878292	1.119370
C	3.483258	1.366182	2.144905
C	4.258667	2.508852	1.979281
C	4.196106	3.226866	0.782844
C	3.374279	2.782854	-0.244948
N	1.832473	-0.256024	1.189133
P	2.171197	-1.682689	2.075147
C	3.971386	-2.303544	1.941471
C	5.157648	-1.345811	2.055453
P	1.297822	-3.084646	-0.090923
C	2.336909	-3.449656	-1.649975
C	1.505134	-3.874290	-2.859046
C	1.797495	-1.550355	3.952103
C	0.349409	-1.105969	4.129168
N	-0.054328	-2.142053	-0.470039
C	-1.369234	-2.659529	-0.486598
C	-1.787873	-3.743188	-1.267898
C	-3.110506	-4.182242	-1.246598
C	-4.047350	-3.505852	-0.463121
C	-3.662912	-2.407729	0.299248
C	-2.323075	-1.978090	0.325028
N	-1.834371	-0.880973	1.015727
C	-2.408262	-0.360084	2.168375
C	-1.996313	0.973359	2.443922
C	-2.460077	1.620549	3.590930
C	-3.311352	0.958587	4.480347

C	-3.687967	-0.358540	4.229884
C	-3.237131	-1.020308	3.085456
N	-1.115937	1.480756	1.484723
P	-1.051638	3.086540	0.837927
C	-0.198409	4.249950	2.098870
C	0.606157	5.308969	1.338960
C	0.940878	-4.773486	0.701739
C	-0.127520	-4.674171	1.792393
U	-0.120428	0.217293	-0.129896
C	-2.570443	2.368111	-3.170617
C	-1.869434	3.002482	-4.370646
C	-2.831585	3.754660	0.978357
C	-2.918904	5.143537	0.340168
C	0.709318	-5.985699	-0.203533
C	3.211524	-2.243986	-1.998692
C	-3.863299	2.802144	0.385370
C	-4.090617	2.398913	-3.365515
C	0.684073	3.504795	3.094120
C	2.728807	-0.756514	4.870526
C	-3.857602	-1.054761	-3.905760
C	4.138677	-3.497960	2.890349
H	-2.141380	2.637475	3.799401
H	-1.064510	-4.236171	-1.908607
H	1.912254	-4.924138	1.197966
H	2.980181	-4.280294	-1.324432
H	-4.402562	-1.862137	0.875233
H	-3.029552	3.850987	2.052822
H	-0.103462	0.893263	-5.159256
H	3.853356	-2.488051	-2.853084
H	3.856637	-1.936803	-1.171403
H	2.603684	-1.380010	-2.280303
H	3.300074	3.346857	-1.168822
H	4.778176	4.135339	0.655227
H	-3.516442	-2.054854	2.914222
H	-2.315821	2.961584	-2.282929
H	-5.086623	-3.823706	-0.457779
H	3.522829	0.827667	3.082617
H	-1.014796	4.742758	2.645285
H	1.871114	-2.611477	4.230738
H	-4.333606	-0.883617	4.928893
H	-2.436796	0.158796	-4.991236
H	-3.409361	-5.031715	-1.854247
H	-3.664763	1.471238	5.370636
H	0.124905	2.762936	3.669667

H	1.130175	4.217354	3.799581
H	1.504164	2.988170	2.589364
H	3.970791	-2.693455	0.915680
H	4.086219	1.845740	-5.032514
H	2.004672	1.440797	-6.333871
H	4.896820	2.847045	2.790997
H	-0.253738	-5.931258	-0.715255
H	0.699466	-6.891939	0.414824
H	1.498022	-6.113539	-0.949486
H	3.787956	-0.975837	4.711427
H	2.497635	-1.000423	5.915572
H	2.575696	0.320200	4.756358
H	0.215793	-0.066809	3.816905
H	0.055414	-1.177562	5.182563
H	-0.348418	-1.710994	3.545153
H	4.051046	1.711100	-2.561303
H	1.445471	4.846770	0.809198
H	1.016403	6.050258	2.035967
H	0.003749	5.846578	0.599771
H	-3.713525	2.669341	-0.687475
H	-4.870842	3.211582	0.530585
H	-3.830805	1.816732	0.854171
H	0.022148	-3.801224	2.433008
H	-0.090343	-5.569191	2.424582
H	-1.128064	-4.606005	1.360254
H	0.949575	-4.799633	-2.691243
H	2.164137	-4.035575	-3.721481
H	0.795843	-3.086837	-3.125669
H	-2.258458	5.869867	0.822931
H	-3.942176	5.529786	0.421790
H	-2.662502	5.112708	-0.724986
H	-3.893749	-1.695194	-3.018340
H	-4.137836	-1.665172	-4.773382
H	-4.619650	-0.280206	-3.788554
H	-4.376444	1.918518	-4.307581
H	-4.442403	3.436298	-3.415983
H	-4.635370	1.901879	-2.556466
H	-0.425679	-1.250505	-4.445396
H	-1.728868	-2.234161	-5.136362
H	-1.434056	-2.259171	-3.394187
H	-0.794251	3.101747	-4.217653
H	-2.280326	4.006001	-4.544068
H	-2.033584	2.429749	-5.290433
H	4.233735	-3.177235	3.932371

H	5.052278	-4.047619	2.635771
H	3.303472	-4.204341	2.835017
H	5.104249	-0.530760	1.332980
H	6.082413	-1.906775	1.866916
H	5.245483	-0.904265	3.051873

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C	7.451592	15.252895	-0.458854
C	6.251243	14.956309	0.200313
C	5.077984	14.738913	-0.584532
C	5.142629	14.889558	-1.970530
C	6.343361	15.222596	-2.606143
C	7.496736	15.391592	-1.849577
N	3.970330	14.329294	0.159856
P	2.379144	13.817309	-0.256877
C	2.488036	12.589505	-1.704852
C	3.642675	11.615349	-1.494403
N	6.079014	14.735572	1.566037
C	6.929840	15.221345	2.534134
C	6.890330	14.558187	3.801255
C	7.663364	15.036793	4.863355
C	8.517618	16.128723	4.711654
C	8.556676	16.785692	3.482438
C	7.768145	16.351825	2.422445
N	5.982787	13.464909	3.914156
P	6.413031	12.020235	4.563911
C	8.272982	11.774901	4.804617
C	8.632289	10.411110	5.394254
P	5.379675	10.512444	3.092698
C	6.693181	10.146354	1.795211
C	6.307375	8.965053	0.901176
C	5.612155	11.699482	6.239553
C	4.153940	12.159378	6.209374
N	4.138203	11.409032	2.500461
C	2.820883	10.889624	2.336967
C	2.533682	9.720646	1.626977
C	1.223519	9.270365	1.463508
C	0.179659	10.032449	1.987023
C	0.439519	11.218208	2.665925
C	1.756960	11.678916	2.875259
N	2.125390	12.865275	3.470411
C	1.353978	13.543342	4.410486
C	1.735397	14.905753	4.611771
C	1.051284	15.671504	5.559883

C	0.021252	15.120795	6.329479
C	-0.318792	13.783374	6.167555
C	0.347480	13.000284	5.220436
N	2.826615	15.316209	3.838292
P	3.559207	16.876423	3.664580
C	4.044134	17.510074	5.406154
C	5.236531	18.463151	5.274489
C	4.889556	8.846849	3.842309
C	6.081846	8.051283	4.372535
U	3.992203	13.931444	2.422794
C	1.404584	15.299919	-0.975707
C	1.495438	15.578161	-2.475183
C	2.146589	18.077939	3.223291
C	2.645781	19.521668	3.158132
C	3.753091	8.915467	4.862360
C	6.945683	11.396689	0.951097
C	1.533029	17.649335	1.896085
C	-0.057688	15.192126	-0.527403
C	4.384154	16.364923	6.355663
C	6.363325	12.388246	7.382450
C	1.150572	11.856476	-1.835199
C	9.124919	12.104242	3.578998
H	1.339662	16.706024	5.716529
H	3.349826	9.161638	1.175765
H	4.501193	8.340420	2.950594
H	7.591710	9.886257	2.370081
H	-0.386084	11.825730	3.019249
H	1.382246	17.999806	4.004799
H	4.247358	14.727220	-2.560657
H	6.074219	11.613692	0.329009
H	7.798779	11.221472	0.287094
H	7.143398	12.295736	1.538248
H	7.772256	16.904825	1.490075
H	9.189234	17.660193	3.351493
H	0.092809	11.949506	5.125359
H	1.868726	16.134886	-0.438059
H	-0.850674	9.715318	1.845927
H	7.582695	14.556039	5.834889
H	3.182536	18.062137	5.806997
H	5.668506	10.611165	6.375670
H	-1.101175	13.336517	6.775953
H	2.672305	13.155103	-2.625056
H	1.026009	8.353015	0.916623
H	-0.495726	15.738977	7.058674

H	3.527794	15.708679	6.527735
H	4.708288	16.767011	7.324551
H	5.208759	15.767074	5.953651
H	8.473249	12.545860	5.557981
H	8.441516	15.628987	-2.332214
H	6.368124	15.336507	-3.686685
H	9.116891	16.473465	5.549195
H	4.078370	9.338334	5.815880
H	3.406564	7.895079	5.060816
H	2.902096	9.489921	4.493380
H	7.399657	12.057572	7.492196
H	5.846975	12.164700	8.322344
H	6.349829	13.475546	7.263908
H	4.098143	13.245406	6.098760
H	3.668808	11.890531	7.153706
H	3.573426	11.731331	5.390292
H	8.366367	15.358250	0.115812
H	6.114951	17.929993	4.896857
H	5.494038	18.888644	6.253172
H	5.040624	19.296885	4.594142
H	2.259828	17.750762	1.081555
H	0.664557	18.272718	1.650108
H	1.201623	16.608191	1.931433
H	6.901040	7.968001	3.652384
H	5.751605	7.033972	4.609746
H	6.479460	8.481378	5.296213
H	6.185501	8.023391	1.443107
H	7.098611	8.815687	0.158444
H	5.387074	9.175242	0.348468
H	2.959853	19.899645	4.135487
H	1.847438	20.181142	2.795366
H	3.491620	19.620193	2.466968
H	0.914075	11.300972	-0.921387
H	1.189497	11.140344	-2.665831
H	0.320432	12.541488	-2.035044
H	-0.579237	14.375491	-1.039500
H	-0.598471	16.117972	-0.759522
H	-0.141298	15.008704	0.547463
H	4.605210	12.133238	-1.516233
H	3.645635	10.858108	-2.289004
H	3.542956	11.095770	-0.535456
H	2.519805	15.774953	-2.800221
H	0.898672	16.465078	-2.725219
H	1.097010	14.750956	-3.073174

H	9.058181	11.332982	2.808001
H	10.173278	12.157637	3.893488
H	8.859541	13.066982	3.139166
H	8.070674	10.166893	6.300625
H	9.695201	10.409030	5.659858
H	8.482091	9.605129	4.670568

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