Supporting Information Appendix

for

Identification of a Uranium-Rhodium Triple Bond in a Heterometallic Cluster

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1. Materials and Methods

General information: All reactions were carried out using a Vigor Ar-atmosphere glove box (<1 ppm O_2/H_2O). Solvents were dried and degassed before use through a Mikrouna solvent drying system. Samples were carefully checked for purity and reproducibility of their data. Elemental analyses (C, H, N) were performed on a Vario EL III elemental analyser at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences. The powder X-ray diffraction pattern (PXRD) measurements were carried out on a Philips X'pert MPD Pro X-ray diffractometer using Cu Kα radiation (λ = 0.15418 nm), and the X-ray tube was operated at 40 kV and 40 mA at room temperature. Magnetic susceptibility measurements on crystalline samples were carried out on a SQUID magnetometer at 0.1 T in the temperature range from 5 to 300 K. Absorption spectra were recorded on a Lambda 750 spectrometer at room temperature. X-ray photoelectron spectroscopy (XPS) measurements were carried out on an Axis Ultra imaging photoelectron spectrometer. Fourier Transform Infrared Spectra (FT-IR) (4000-400 cm^{-1}) were collected on a Nicolet FT-IR 170X spectrophotometer at 25 °C using KBr plates. Complex **1** was synthesized according to a published method (1).

Preparation of Complex 2

Complex **1** (284.0 mg, 0.37 mmol) was dissolved in a 20 mL vial with THF (5 mL), then a solution of $[RhCl(COD)]_2$ (183.0 mg, 0.37 mmol) in THF (5 mL) was added dropwise at room temperature. After shaking serval times, the resulting mixture was allowed to stand undisturbed. Complex **2** was precipitated as brown crystals from the THF solution within 24 h at the same temperature. Separation of the target crystals was easier with purer precursor. The solvent was decanted and replaced twice with fresh THF. Pure crystalline **2** was obtained in 58% yield (261.0 mg). The recording of NMR spectra of **2** were prevented by its poor solubility. Therefore, the elemental analysis and powder X-ray diffraction were used to confirm the purity of the bulk samples. FT-IR (cm^{-1}): 2953 (s), 2866 (s), 1460 (m), 1381 (w), 1340 (w), 1239 (w), 1158 (m), 1129 (m), 1078 (m), 928(m), 769 (m), 653 (m), 549 (m). Anal. Calcd (%) for $C_{64}H_{132}Cl_6N_8P_6Rh_4U_2$: C, 33.42; H, 5.78; N, 4.87; Found: C, 33.81; H, 5.58; N, 4.43.

Preparation of Complex 3

KC_8 (48.7 mg 0.36 mmol) was added to a suspension of **2** (147.0 mg, 0.06 mmol) in THF (5 ml) at ambient temperature. The mixture was stirred overnight. After removing THF *in vacuo*, the residual solid was extracted with toluene. Black crystals were grown from toluene solution at –35 °C in 2 days. Washing with cooled toluene afforded pure crystalline **3** in 26% yield (31.0 mg). The recording of NMR spectra of **3** were prevented by its poor solubility and the elemental analysis and powder X-ray diffraction were used to confirm the purity of the bulk samples. FT-IR (cm^{-1}): 2914 (s), 2831 (s), 1450 (w), 1369 (w), 1232 (w), 1181 (m), 1020 (w), 912 (w), 752 (s), 630 (m), 536(m). Anal. Calcd (%) for $C_{55}H_{116}N_8P_6Rh_4U_2$: C, 33.65; H, 5.96; N, 5.71; Found: C, 33.40; H, 5.86; N, 5.63.

2. Supporting Figures

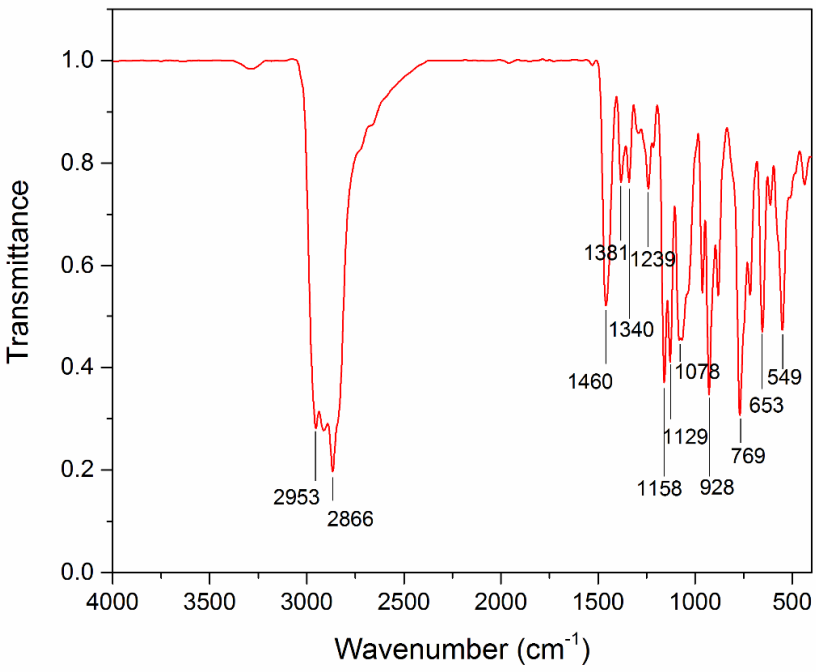

Fig. S1. FT-IR spectrum of complex **2**

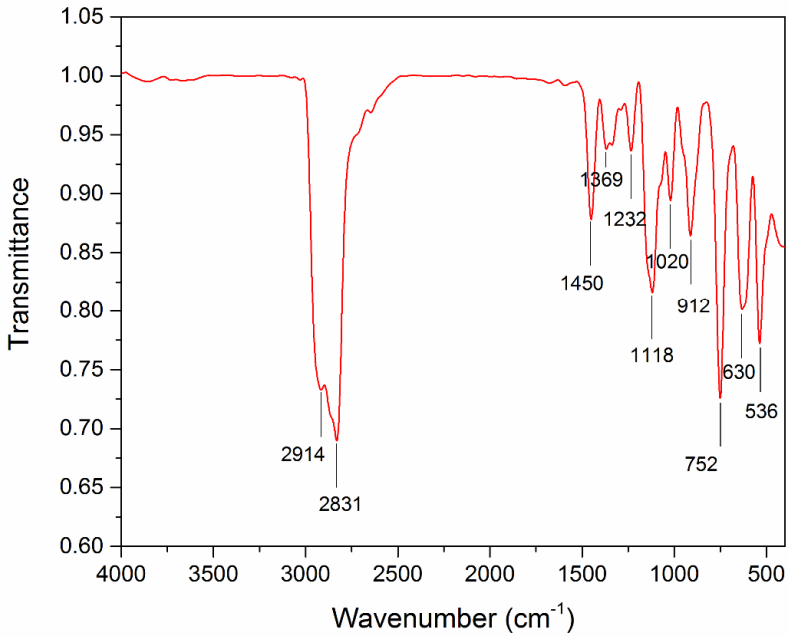

Fig. S2. FT-IR spectrum of complex **3**.

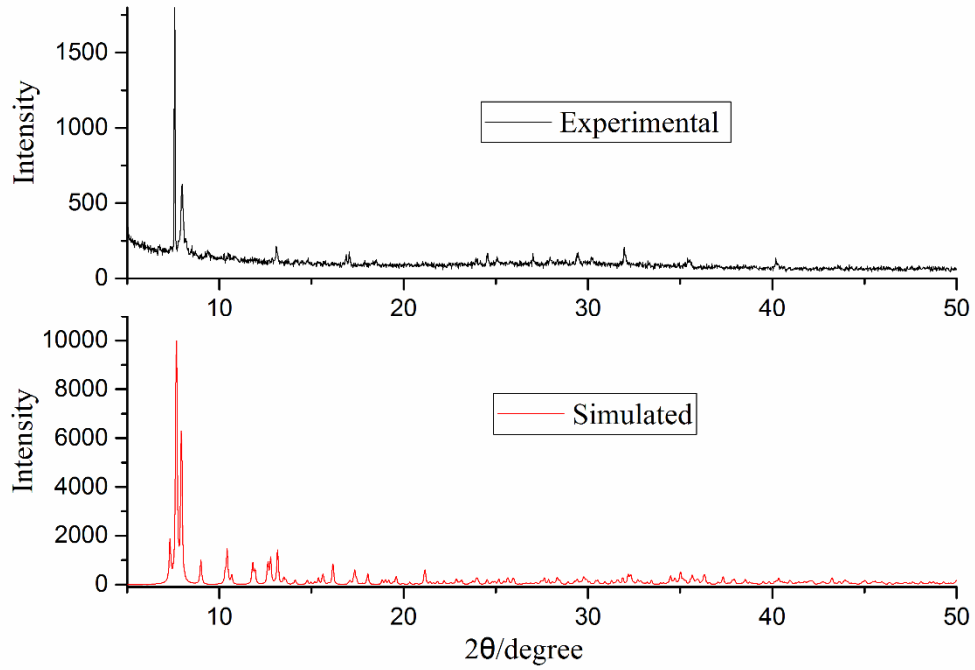

Fig. S3. PXRD patterns of **2** in the range from 5 to 50 degree.

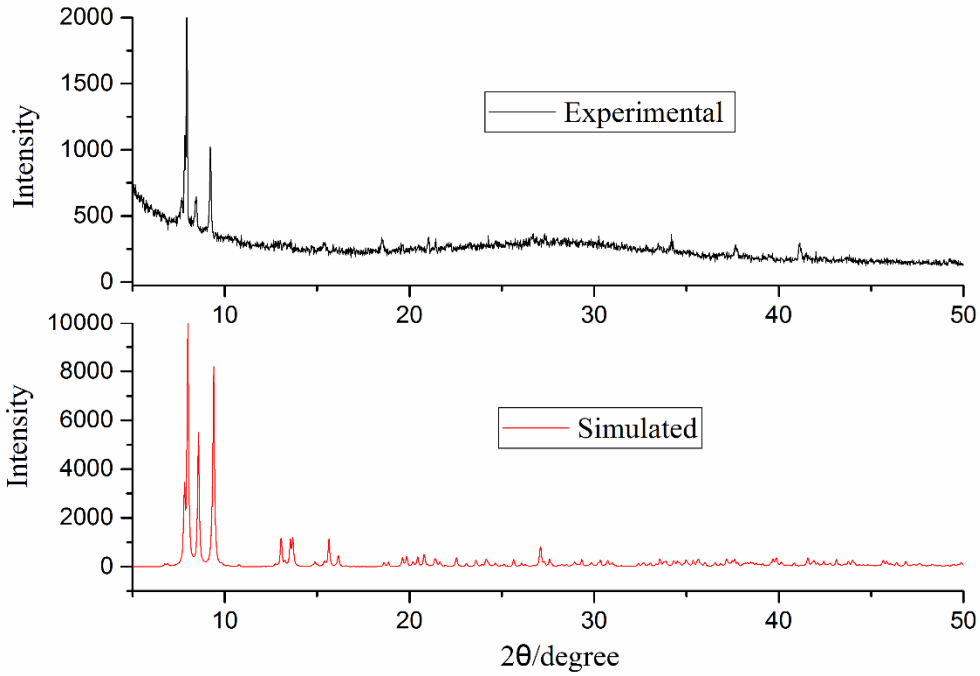

Fig. S4. PXRD patterns of **3** in the range from 5 to 50 degree.

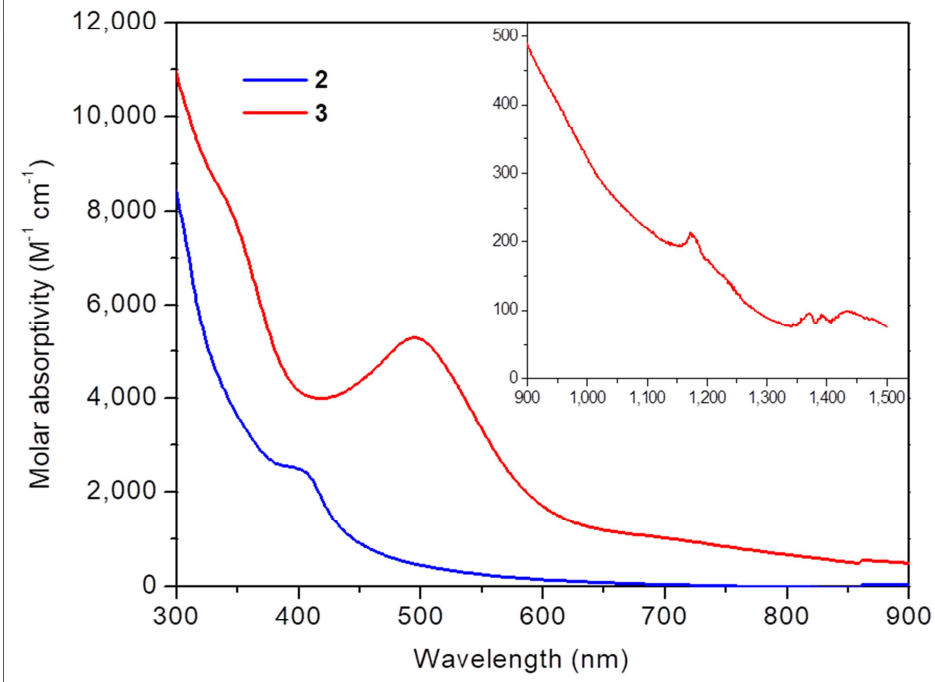

Fig. S5. UV-visible absorption spectra for **2** and **3** measured in tetrahydrofuran at room temperature. Inset: Near infrared absorption spectrum of complex **3**.

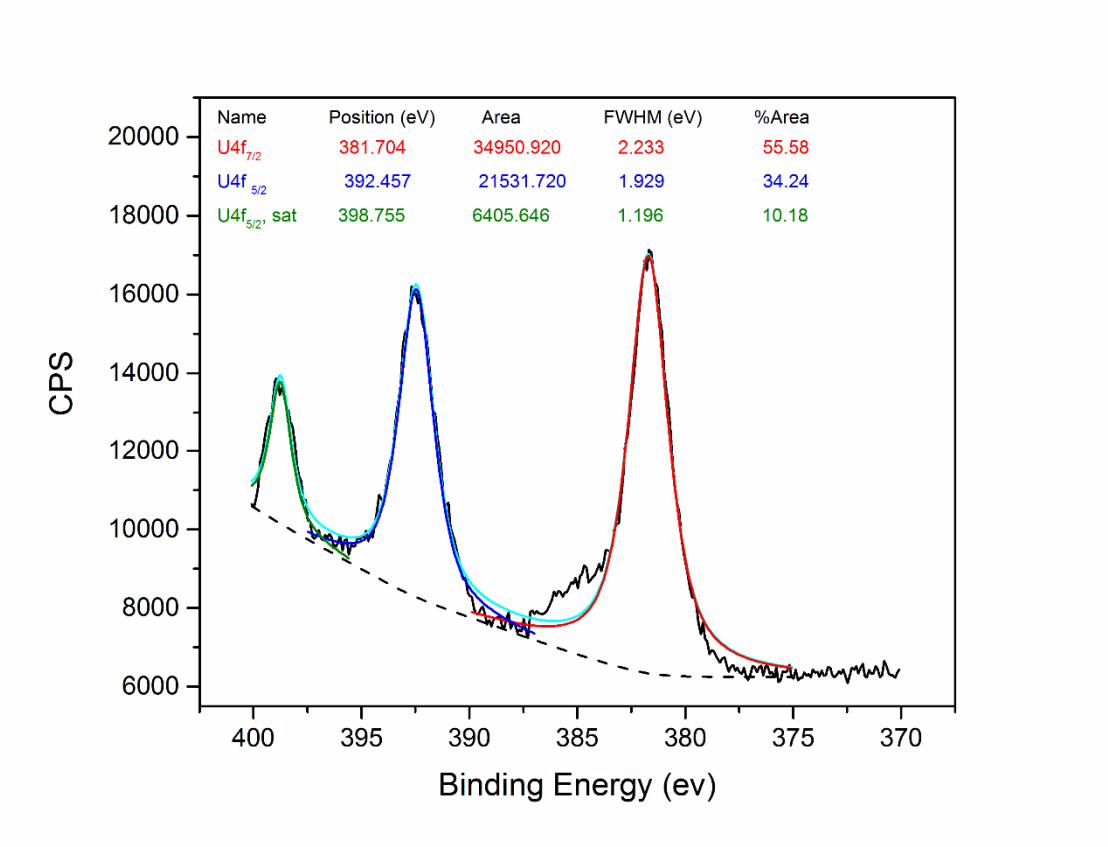

Fig. S6. XPS spectrum of U4f of complex **2**

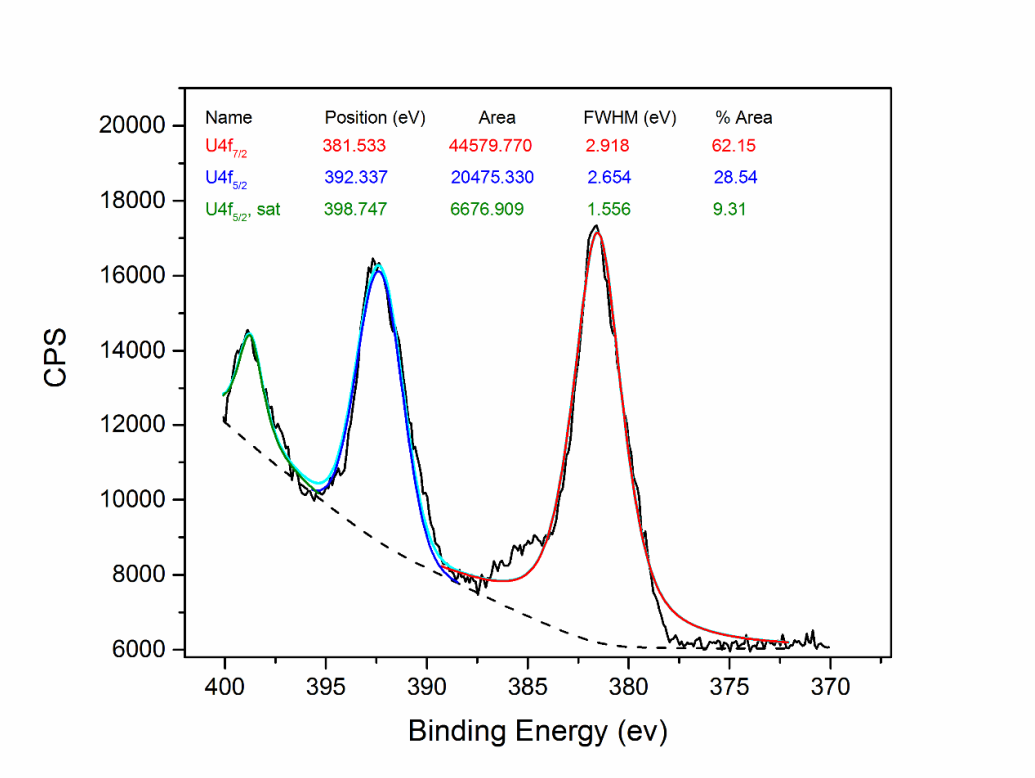

Fig. S7. XPS spectrum of U4f of complex **3**.

3. Single-Crystal X-Ray Diffraction Experiment

Single-crystal X-ray diffraction data for complexes **2** and **3** were collected at 123 K on a Bruker D8 CMOS detector using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). Integrations, cell refinement and data reduction were performed with the SAINT program (2). All structures were solved by direct methods and refined on F^2 using full-matrix least-squares methods with SHELXTL version 6.10 (3). All non-hydrogen atoms were refined on F^2 by full-matrix least-squares procedures with the use of anisotropic displacement parameters. All calculations were carried out with the SHELXTL PC program package. In complex **2**, fixed distance (DFIX) and pseudo-isotropic (ISOR) restraints were applied for the refinement of the disordered atoms. Similarity restraint (DELU) was used to constrain the displacement ellipsoids of the atoms. In complex **3**, the integral structure, including the heavy atoms, was disordered. Two alternative orientations for the heavy atoms and ligand were refined and resulted in site occupancies of 87.5% and 12.5%, respectively. Fixed distance (DFIX) was used to rationalize the bond parameters of the ligand. SIMU, DELU and ISOR restraints were applied for the refinement of the disordered ligand atoms. Evaluation of the CIF using the CheckCIF routine at www.checkcif.iucr.org gave no A or B alert for complexes **2** and **3**. Details of the data collection and refinement for complexes **2** and **3** are given in Table S1. CCDC-1886167 (**2**) and 1886168 (**3**) contain the crystallographic data reported in 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 structure refinements for complexes **2** and **3**

Complex	**2**	**3**
Formula	$(C_{36}H_{74}Cl_3N_4OP_3Rh_2U)_2$	$C_{55}H_{116}N_8P_6Rh_4U_2$
*M*r [g/mol]	2444.21	1963.07
Temp. [K]	123(2)	123(2)
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
a [Å]	15.6600(6)	13.1220(10)
b [Å]	13.1065(5)	13.5533(10)
c [Å]	25.2326(10	38.271(3)
α [°]	90	90
β [°]	107.0390(10)	95.674(2)
γ [°]	90	90
Volume [$Å^3$]	4951.6(3)	6773.0(9)
$Z/D_{calcd.}$[g/cm^3]	4/ 1.639	4/1.925
μ[mm^{-1}]	4.210	5.899
F(000)	2416	3824
θ range/deg	2.065 to 25.020	2.139 to 26.000
Index ranges	$-18 \le h \le 14$	$-16 \le h \le 12$
	$-15 \le k \le 15$	$-16 \le k \le 16$

	$-30 \leq l \leq 30$	$-47 \leq l \leq 47$
Collected data	35239	47955
Unique data	8748 [R(int) = 0.0564]	13278 [R(int) = 0.0703]
Completeness	99.9 %	99.7 %
Data/parameters	8748 / 466	13278 / 1223
GOF on F^2	1.052	1.034
Final R indices [I>2σ(*I*)]	$R_1 = 0.0503$	$R_1 = 0.0613$
	$wR_2 = 0.1235$	$wR_2 = 0.1462$
R indices (all data)	$R_1 = 0.0697$	$R_1 = 0.0711$
	$wR_2 = 0.1334$	$wR_2 = 0.1523$
Largest diff. peak and hole [e·Å^{-3}]	2.261 and -1.162	3.180 and -2.815

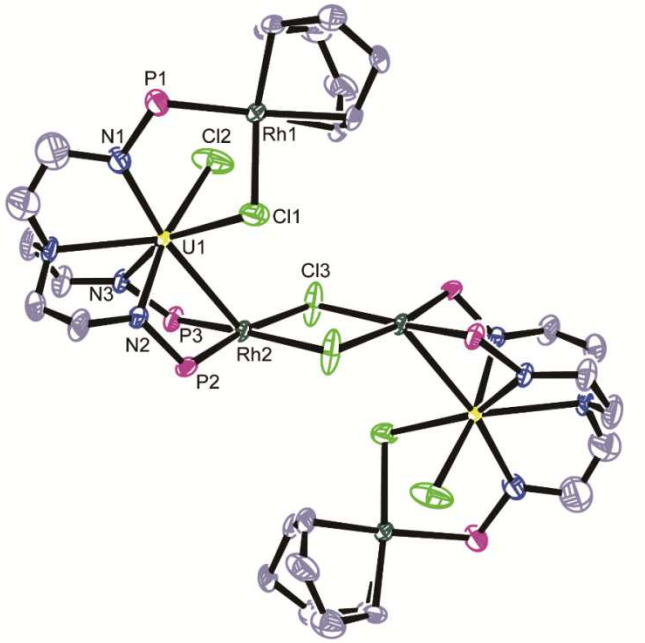

Fig. S8. Crystal structure of complex **2**. Thermal ellipsoids are drawn at 50% probability. Hydrogen atoms and isopropyl moieties in P^iPr_2 are omitted for clarity.

Table S2 Bond lengths (Å) and angles [°] for complex **2**

C(1)-C(2)	1.387(13)	C(1)-N(4)	1.467(14)
C(2)-N(1)	1.517(15)	C(3)-N(4)	1.444(13)
C(3)-C(4)	1.499(15)	C(4)-N(2)	1.459(11)
C(5)-N(4)	1.477(13)	C(5)-C(6)	1.490(14)
C(6)-N(3)	1.442(11)	C(11)-C(12)	1.347(16)
C(11)-C(18)	1.522(17)	C(11)-Rh(1)	2.192(9)
C(12)-C(13)	1.520(14)	C(12)-Rh(1)	2.228(9)
C(13)-C(14)	1.525(15)	C(14)-C(15)	1.524(14)
C(15)-C(16)	1.409(13)	C(15)-Rh(1)	2.099(8)

C(16)-C(17)	1.501(14)	C(16)-Rh(1)	2.103(9)
C(17)-C(18)	1.536(15)	C(19)-C(20)	1.47(2)
C(19)-C(21)	1.549(16)	C(19)-P(1)	1.845(12)
C(22)-C(23)	1.515(16)	C(22)-C(24)	1.534(19)
C(22)-P(1)	1.876(12)	C(25)-C(26)	1.501(14)
C(25)-C(27)	1.549(13)	C(25)-P(3)	1.906(10)
C(28)-C(30)	1.519(14)	C(28)-C(29)	1.548(15)
C(28)-P(3)	1.865(10)	C(31)-C(33)	1.471(12)
C(31)-C(32)	1.472(12)	C(31)-P(2)	1.870(10)
C(34)-C(36)	1.515(12)	C(34)-C(35)	1.542(14)
C(34)-P(2)	1.869(10)	O(1)-C(40)	1.4433
Cl(1)-Rh(1)	2.431(3)	Cl(1)-U(1)	2.780(2)
Cl(2)-U(1)	2.686(3)	Cl(3)-Rh(2)	2.391(2)
Cl(3)-Rh(2)#1	2.416(2)	N(1)-P(1)	1.672(8)
N(1)-U(1)	2.347(8)	N(2)-P(2)	1.651(7)
N(2)-U(1)	2.265(7)	N(3)-P(3)	1.665(7)
N(3)-U(1)	2.280(7)	N(4)-U(1)	2.652(7)
P(1)-Rh(1)	2.326(3)	P(2)-Rh(2)	2.282(2)
P(2)-U(1)	3.119(2)	P(3)-Rh(2)	2.276(2)
P(3)-U(1)	3.111(2)	Rh(2)-Cl(3)#1	2.416(2)
Rh(2)-U(1)	2.9609(7)		
C(2)-C(1)-N(4)	119.2(11)	C(1)-C(2)-N(1)	111.5(11)
N(4)-C(3)-C(4)	112.6(9)	N(2)-C(4)-C(3)	108.0(8)
N(4)-C(5)-C(6)	111.5(8)	N(3)-C(6)-C(5)	108.6(8)
C(12)-C(11)-C(18)	125.7(10)	C(12)-C(11)-Rh(1)	73.7(6)
C(18)-C(11)-Rh(1)	107.2(7)	C(11)-C(12)-C(13)	123.7(12)
C(11)-C(12)-Rh(1)	70.8(6)	C(13)-C(12)-Rh(1)	111.8(7)
C(12)-C(13)-C(14)	111.6(9)	C(15)-C(14)-C(13)	112.4(9)
C(16)-C(15)-C(14)	126.1(9)	C(16)-C(15)-Rh(1)	70.6(5)
C(14)-C(15)-Rh(1)	111.7(6)	C(15)-C(16)-C(17)	124.7(9)
C(15)-C(16)-Rh(1)	70.3(5)	C(17)-C(16)-Rh(1)	115.3(7)
C(16)-C(17)-C(18)	111.7(9)	C(11)-C(18)-C(17)	113.9(10)
C(20)-C(19)-C(21)	110.3(14)	C(20)-C(19)-P(1)	111.0(9)
C(21)-C(19)-P(1)	113.9(9)	C(23)-C(22)-C(24)	110.3(11)
C(23)-C(22)-P(1)	121.6(11)	C(24)-C(22)-P(1)	108.9(7)
C(26)-C(25)-C(27)	110.7(9)	C(26)-C(25)-P(3)	117.8(8)
C(27)-C(25)-P(3)	110.9(7)	C(30)-C(28)-C(29)	109.5(9)
C(30)-C(28)-P(3)	111.4(7)	C(29)-C(28)-P(3)	116.5(8)
C(33)-C(31)-C(32)	109.9(9)	C(33)-C(31)-P(2)	111.8(8)
C(32)-C(31)-P(2)	119.0(9)	C(36)-C(34)-C(35)	110.2(8)
C(36)-C(34)-P(2)	116.3(7)	C(35)-C(34)-P(2)	112.8(7)
Rh(1)-Cl(1)-U(1)	91.89(8)	Rh(2)-Cl(3)-Rh(2)#1	102.17(9)
C(2)-N(1)-P(1)	113.4(7)	C(2)-N(1)-U(1)	123.9(7)

P(1)-N(1)-U(1)	122.1(4)	C(4)-N(2)-P(2)	128.6(7)
C(4)-N(2)-U(1)	123.6(6)	P(2)-N(2)-U(1)	104.5(3)
C(6)-N(3)-P(3)	128.7(6)	C(6)-N(3)-U(1)	127.4(6)
P(3)-N(3)-U(1)	103.0(3)	C(3)-N(4)-C(1)	109.4(9)
C(3)-N(4)-C(5)	114.1(9)	C(1)-N(4)-C(5)	108.3(9)
C(3)-N(4)-U(1)	109.5(5)	C(1)-N(4)-U(1)	111.5(6)
C(5)-N(4)-U(1)	104.0(6)	N(1)-P(1)-C(19)	105.5(5)
N(1)-P(1)-C(22)	108.2(5)	C(19)-P(1)-C(22)	103.4(7)
N(1)-P(1)-Rh(1)	110.8(3)	C(19)-P(1)-Rh(1)	115.1(5)
C(22)-P(1)-Rh(1)	113.2(4)	N(2)-P(2)-C(34)	104.3(4)
N(2)-P(2)-C(31)	110.2(4)	C(34)-P(2)-C(31)	107.1(5)
N(2)-P(2)-Rh(2)	108.8(3)	C(34)-P(2)-Rh(2)	111.5(3)
C(31)-P(2)-Rh(2)	114.5(3)	N(2)-P(2)-U(1)	44.7(3)
C(34)-P(2)-U(1)	116.1(4)	C(31)-P(2)-U(1)	133.8(4)
Rh(2)-P(2)-U(1)	64.33(6)	N(3)-P(3)-C(28)	110.8(4)
N(3)-P(3)-C(25)	104.9(4)	C(28)-P(3)-C(25)	107.0(5)
N(3)-P(3)-Rh(2)	107.8(3)	C(28)-P(3)-Rh(2)	114.0(4)
C(25)-P(3)-Rh(2)	112.1(3)	N(3)-P(3)-U(1)	45.6(2)
C(28)-P(3)-U(1)	142.0(4)	C(25)-P(3)-U(1)	108.1(3)
Rh(2)-P(3)-U(1)	64.53(6)	C(15)-Rh(1)-C(16)	39.2(4)
C(15)-Rh(1)-C(11)	96.5(4)	C(16)-Rh(1)-C(11)	81.4(4)
C(15)-Rh(1)-C(12)	80.4(4)	C(16)-Rh(1)-C(12)	88.5(4)
C(11)-Rh(1)-C(12)	35.5(4)	C(15)-Rh(1)-P(1)	91.4(3)
C(16)-Rh(1)-P(1)	97.7(3)	C(11)-Rh(1)-P(1)	165.8(3)
C(12)-Rh(1)-P(1)	158.5(4)	C(15)-Rh(1)-Cl(1)	146.8(3)
C(16)-Rh(1)-Cl(1)	170.5(3)	C(11)-Rh(1)-Cl(1)	89.7(3)
C(12)-Rh(1)-Cl(1)	86.3(3)	P(1)-Rh(1)-Cl(1)	89.98(10)
P(3)-Rh(2)-P(2)	98.77(9)	P(3)-Rh(2)-Cl(3)	91.27(9)
P(2)-Rh(2)-Cl(3)	169.04(9)	P(3)-Rh(2)-Cl(3)#1	166.60(9)
P(2)-Rh(2)-Cl(3)#1	91.61(9)	Cl(3)-Rh(2)-Cl(3)#1	77.83(9)
P(3)-Rh(2)-U(1)	71.53(6)	P(2)-Rh(2)-U(1)	71.68(6)
Cl(3)-Rh(2)-U(1)	116.11(9)	Cl(3)#1-Rh(2)-U(1)	120.20(8)
N(2)-U(1)-N(3)	87.9(3)	N(2)-U(1)-N(1)	103.8(3)
N(3)-U(1)-N(1)	120.6(3)	N(2)-U(1)-N(4)	67.3(2)
N(3)-U(1)-N(4)	65.4(2)	N(1)-U(1)-N(4)	66.6(3)
N(2)-U(1)-Cl(2)	168.49(19)	N(3)-U(1)-Cl(2)	91.5(2)
N(1)-U(1)-Cl(2)	86.3(2)	N(4)-U(1)-Cl(2)	122.69(19)
N(2)-U(1)-Cl(1)	90.0(2)	N(3)-U(1)-Cl(1)	156.84(18)
N(1)-U(1)-Cl(1)	82.2(2)	N(4)-U(1)-Cl(1)	134.02(18)
Cl(2)-U(1)-Cl(1)	86.03(10)	N(2)-U(1)-Rh(2)	74.69(17)
N(3)-U(1)-Rh(2)	74.12(17)	N(1)-U(1)-Rh(2)	165.2(2)
N(4)-U(1)-Rh(2)	124.21(16)	Cl(2)-U(1)-Rh(2)	94.10(7)
Cl(1)-U(1)-Rh(2)	83.08(6)	N(2)-U(1)-P(3)	87.58(19)

N(3)-U(1)-P(3)	31.43(17)	N(1)-U(1)-P(3)	150.6(2)
N(4)-U(1)-P(3)	94.25(17)	Cl(2)-U(1)-P(3)	85.99(8)
Cl(1)-U(1)-P(3)	125.44(7)	Rh(2)-U(1)-P(3)	43.94(4)
N(2)-U(1)-P(2)	30.83(17)	N(3)-U(1)-P(2)	82.52(19)
N(1)-U(1)-P(2)	132.3(2)	N(4)-U(1)-P(2)	92.66(18)
Cl(2)-U(1)-P(2)	137.76(8)	Cl(1)-U(1)-P(2)	83.89(7)
Rh(2)-U(1)-P(2)	44.00(4)	P(3)-U(1)-P(2)	67.48(6)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+2,-z+1

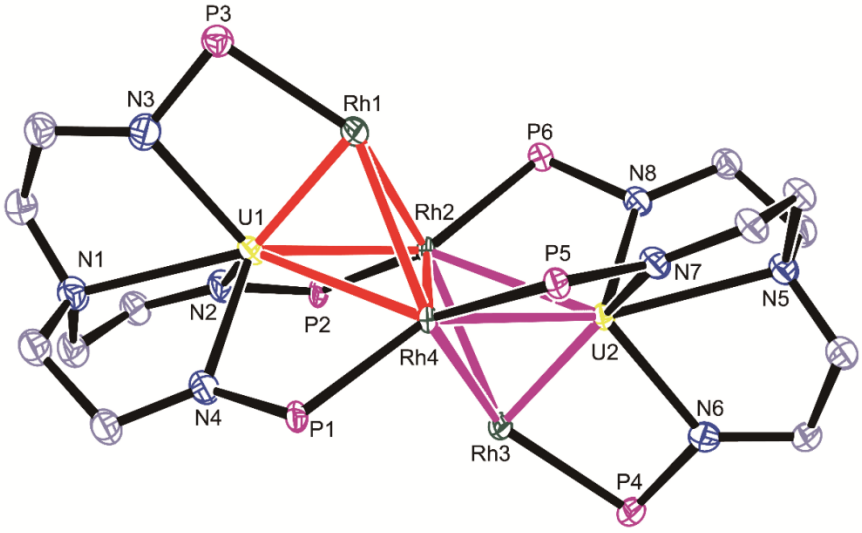

Fig. S9. Crystal structure of complex **3**. Thermal ellipsoids are drawn at 50% probability. Hydrogen atoms and isopropyl moieties in P^iPr_2 are omitted for clarity.

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

U(1)-N(4)	2.281(13)	U(1)-N(4')	2.29(10)
U(1)-N(2')	2.30(9)	U(1)-N(2)	2.312(13)
U(1)-Rh(1)	2.3164(9)	U(1)-N(3)	2.320(9)
U(1)-N(1)	2.655(9)	U(1)-Rh(2')	2.895(9)
U(1)-Rh(4)	2.8976(10)	U(1)-Rh(2)	2.9740(10)
U(1)-Rh(4')	3.038(9)	U(1)-P(3)	3.101(3)
U(2)-N(7)	2.263(10)	U(2)-N(6)	2.301(10)
U(2)-N(8)	2.311(10)	U(2)-Rh(3)	2.3125(10)
U(2)-N(5)	2.645(9)	U(2)-Rh(2)	2.9445(12)
U(2)-Rh(4)	2.9788(11)	U(2)-P(4)	3.082(3)
U(2)-P(5)	3.131(3)	U(2)-P(6)	3.227(3)
Rh(2)-P(5)	2.318(3)	Rh(2)-P(1)	2.359(4)
Rh(2)-Rh(1)	2.8815(14)	Rh(2)-Rh(4)	2.9511(16)
Rh(2)-Rh(3)	3.0317(15)	Rh(3)-P(4)	2.301(3)
Rh(3)-Rh(4)	2.8027(14)	Rh(4)-P(2)	2.324(3)
Rh(4)-P(6)	2.342(3)	Rh(4)-Rh(1)	2.8858(14)

N(6)-C(8)	1.464(12)	N(6)-P(4)	1.663(10)
N(7)-C(10)	1.447(12)	N(7)-P(5)	1.693(10)
N(8)-C(12)	1.451(12)	N(8)-P(6)	1.656(10)
N(5)-C(7)	1.462(13)	N(5)-C(11)	1.467(12)
N(5)-C(9)	1.475(12)	P(4)-C(31)	1.849(11)
P(4)-C(34)	1.864(11)	P(5)-C(40)	1.860(10)
P(5)-C(37)	1.864(11)	P(6)-C(43)	1.860(10)
P(6)-C(46)	1.871(11)	C(7)-C(8)	1.546(13)
C(9)-C(10)	1.547(13)	C(11)-C(12)	1.540(13)
P(2)-N(2)	1.648(14)	P(2)-C(22)	1.867(11)
P(2)-C(19)	1.869(10)	P(1)-N(4)	1.699(13)
P(1)-C(16)	1.848(11)	P(1)-C(13)	1.869(11)
N(4)-C(2)	1.456(12)	C(1)-N(1)	1.471(13)
C(1)-C(2)	1.537(14)	N(2)-C(4)	1.455(12)
C(3)-N(1)	1.462(12)	C(3)-C(4)	1.539(14)
C(5)-N(1)	1.453(13)	C(5)-C(6)	1.548(13)
C(6)-N(3)	1.450(12)	C(13)-C(14)	1.518(14)
C(13)-C(15)	1.550(13)	C(16)-C(18)	1.530(13)
C(16)-C(17)	1.535(14)	C(19)-C(21)	1.534(13)
C(19)-C(20)	1.544(13)	C(22)-C(24)	1.530(13)
C(22)-C(23)	1.537(12)	C(31)-C(33)	1.525(13)
C(31)-C(32)	1.534(13)	C(34)-C(36)	1.527(13)
C(34)-C(35)	1.537(14)	C(37)-C(39)	1.539(12)
C(37)-C(38)	1.548(13)	C(40)-C(42)	1.526(13)
C(40)-C(41)	1.531(13)	C(43)-C(45)	1.530(13)
C(43)-C(44)	1.540(13)	C(46)-C(48)	1.541(13)
C(46)-C(47)	1.544(12)	U(2')-N(6')	2.29(7)
U(2')-Rh(3')	2.328(7)	U(2')-N(7')	2.36(7)
U(2')-N(8')	2.40(7)	U(2')-N(5')	2.68(2)
U(2')-Rh(4')	2.954(11)	U(2')-Rh(2')	3.010(10)
U(2')-P(4')	3.04(2)	U(2')-P(6')	3.07(2)
U(2')-P(5')	3.18(2)	Rh(2')-P(1')	2.36(3)
Rh(2')-P(5')	2.39(2)	Rh(2')-Rh(3')	2.808(12)
Rh(2')-Rh(4')	2.967(12)	Rh(2')-Rh(1)	3.009(9)
Rh(3')-P(4')	2.32(2)	Rh(3')-Rh(4')	2.908(12)
Rh(4')-P(2')	2.37(3)	Rh(4')-P(6')	2.38(2)
Rh(4')-Rh(1)	2.820(9)	P(5')-N(7')	1.59(7)
P(5')-C(37')	1.85(2)	P(5')-C(40')	1.85(2)
N(5')-C(7')	1.45(2)	N(5')-C(11')	1.45(2)
N(5')-C(9')	1.45(2)	C(9')-C(10')	1.55(2)
C(10')-N(7')	1.45(2)	C(7')-C(8')	1.55(2)
C(8')-N(6')	1.45(2)	N(6')-P(4')	1.68(7)
P(4')-C(31')	1.85(2)	P(4')-C(34')	1.86(2)

P(4')-C(32')	2.36(7)	P(6')-N(8')	1.59(7)
P(6')-C(46')	1.85(2)	P(6')-C(43')	1.85(2)
N(8')-C(12')	1.46(2)	C(12')-C(11')	1.55(2)
C(13')-C(14')	1.55(2)	C(13')-C(15')	1.55(2)
C(13')-P(1')	1.86(2)	C(16')-C(18')	1.54(2)
C(16')-C(17')	1.55(2)	C(16')-P(1')	1.85(2)
C(19')-C(21')	1.54(2)	C(19')-C(20')	1.55(2)
C(19')-P(2')	1.85(2)	C(22')-C(23')	1.55(2)
C(22')-C(24')	1.56(2)	C(22')-P(2')	1.85(2)
P(2')-N(2')	2.09(9)	P(1')-N(4')	1.37(10)
P(1')-C(2')	2.33(7)	N(4')-C(2')	1.46(2)
C(1')-N(1)	1.45(2)	C(1')-C(2')	1.55(2)
C(3')-N(1)	1.46(2)	C(3')-C(4')	1.55(2)
C(4')-N(2')	1.45(2)	C(5')-N(1)	1.45(2)
C(5')-C(6')	1.56(2)	C(6')-N(3)	1.46(2)
C(31')-C(33')	1.54(2)	C(31')-C(32')	1.55(2)
C(34')-C(36')	1.55(2)	C(34')-C(35')	1.55(2)
C(37')-C(38')	1.54(2)	C(37')-C(39')	1.55(2)
C(40')-C(42')	1.35(2)	C(40')-C(41')	1.55(2)
C(43')-C(45')	1.55(2)	C(43')-C(44')	1.55(2)
C(46')-C(48')	1.55(2)	C(46')-C(47')	1.55(2)
Rh(1)-P(3)	2.295(3)	P(3)-N(3)	1.652(9)
P(3)-C(25)	1.873(12)	P(3)-C(28)	1.892(12)
C(25)-C(27)	1.486(17)	C(25)-C(26)	1.538(16)
C(28)-C(30)	1.418(14)	C(28)-C(29)	1.527(17)
C(49)-C(50)	1.34(2)	C(49)-C(54)	1.41(2)
C(50)-C(51)	1.41(2)	C(51)-C(52)	1.41(2)
C(52)-C(53)	1.37(2)	C(52)-C(55)	1.53(2)
C(53)-C(54)	1.37(2)		
N(4')-U(1)-N(2')	114(3)	N(4)-U(1)-N(2)	101.9(4)
N(4)-U(1)-Rh(1)	129.3(3)	N(4')-U(1)-Rh(1)	126(2)
N(2')-U(1)-Rh(1)	119(2)	N(2)-U(1)-Rh(1)	125.2(3)
N(4)-U(1)-N(3)	106.3(4)	N(4')-U(1)-N(3)	97(2)
N(2')-U(1)-N(3)	100(2)	N(2)-U(1)-N(3)	107.7(4)
Rh(1)-U(1)-N(3	78.6(2)	N(4)-U(1)-N(1)	66.9(4)
N(4')-U(1)-N(1)	63(2)	N(2')-U(1)-N(1)	67(2)
N(2)-U(1)-N(1)	66.9(4)	Rh(1)-U(1)-N(1)	144.72(19)
N(3)-U(1)-N(1)	66.2(3)	N(4')-U(1)-Rh(2')	70(2)
N(2')-U(1)-Rh(2')	136(2)	Rh(1)-U(1)-Rh(2')	69.51(17)
N(3)-U(1)-Rh(2')	123.5(3)	N(1)-U(1)-Rh(2')	132.9(3)
N(4)-U(1)-Rh(4)	118.5(3)	N(2)-U(1)-Rh(4)	73.5(3)
Rh(1)-U(1)-Rh(4)	66.12(3)	N(3)-U(1)-Rh(4)	134.1(2)

N(1)-U(1)-Rh(4)	140.02(19)	N(4)-U(1)-Rh(2)	75.2(3)
N(2)-U(1)-Rh(2)	122.6(3)	Rh(1)-U(1)-Rh(2)	64.61(3)
N(3)-U(1)-Rh(2)	128.5(2)	N(1)-U(1)-Rh(2)	142.10(19)
Rh(4)-U(1)-Rh(2)	60.33(3)	N(4')-U(1)-Rh(4')	120(2)
N(2')-U(1)-Rh(4')	85(2)	Rh(1)-U(1)-Rh(4')	61.83(15)
N(3)-U(1)-Rh(4')	136.6(3)	N(1)-U(1)-Rh(4')	148.7(2)
Rh(2')-U(1)-Rh(4')	60.0(2)	N(4)-U(1)-P(3)	126.3(3)
N(4')-U(1)-P(3)	117(2)	N(2')-U(1)-P(3)	109(2)
N(2)-U(1)-P(3)	118.9(3)	Rh(1)-U(1)-P(3)	47.45(5)
N(3)-U(1)-P(3)	31.5(2)	N(1)-U(1)-P(3)	97.3(2)
Rh(2')-U(1)-P(3)	105.73(18)	Rh(4)-U(1)-P(3)	106.19(6)
Rh(2)-U(1)-P(3)	105.85(5)	Rh(4')-U(1)-P(3)	106.06(16)
N(7)-U(2)-N(6)	103.1(4)	N(7)-U(2)-N(8)	106.0(3)
N(6)-U(2)-N(8)	106.5(4)	N(7)-U(2)-Rh(3)	136.0(2)
N(6)-U(2)-Rh(3)	79.8(2)	N(8)-U(2)-Rh(3)	115.3(2)
N(7)-U(2)-N(5)	66.0(3)	N(6)-U(2)-N(5)	65.7(3)
N(8)-U(2)-N(5)	67.9(3)	Rh(3)-U(2)-N(5)	143.9(2)
N(7)-U(2)-Rh(2)	75.8(2)	N(6)-U(2)-Rh(2)	128.5(3)
N(8)-U(2)-Rh(2)	123.6(3)	Rh(3)-U(2)-Rh(2)	69.24(3)
N(5)-U(2)-Rh(2)	141.8(2)	N(7)-U(2)-Rh(4)	119.8(2)
N(6)-U(2)-Rh(4)	135.8(3)	N(8)-U(2)-Rh(4)	73.1(2)
Rh(3)-U(2)-Rh(4)	62.48(3)	N(5)-U(2)-Rh(4)	140.2(2)
Rh(2)-U(2)-Rh(4)	59.76(3)	N(7)-U(2)-P(4)	125.6(3)
N(6)-U(2)-P(4)	32.0(2)	N(8)-U(2)-P(4)	114.2(3)
Rh(3)-U(2)-P(4)	47.92(6)	N(5)-U(2)-P(4)	96.8(2)
Rh(2)-U(2)-P(4)	107.55(7)	Rh(4)-U(2)-P(4)	106.14(6)
N(7)-U(2)-P(5)	31.7(2)	N(6)-U(2)-P(5)	115.2(3)
N(8)-U(2)-P(5)	124.6(3)	Rh(3)-U(2)-P(5)	106.88(6)
N(5)-U(2)-P(5)	97.5(2)	Rh(2)-U(2)-P(5)	44.73(6)
Rh(4)-U(2)-P(5)	98.09(6)	P(4)-U(2)-P(5)	120.63(9)
N(7)-U(2)-P(6)	113.8(3)	N(6)-U(2)-P(6)	127.6(3)
N(8)-U(2)-P(6)	29.3(3)	Rh(3)-U(2)-P(6)	96.50(6)
N(5)-U(2)-P(6)	96.3(2)	Rh(2)-U(2)-P(6)	96.84(6)
Rh(4)-U(2)-P(6)	44.12(5)	P(4)-U(2)-P(6)	119.33(8)
P(5)-U(2)-P(6)	115.82(8)	P(5)-Rh(2)-P(1)	118.09(12)
P(5)-Rh(2)-Rh(1)	102.13(8)	P(1)-Rh(2)-Rh(1)	108.31(9)
P(5)-Rh(2)-U(2)	71.90(8)	P(1)-Rh(2)-U(2)	145.70(9)
Rh(1)-Rh(2)-U(2)	100.48(4)	P(5)-Rh(2)-Rh(4)	121.84(9)
P(1)-Rh(2)-Rh(4)	120.07(9)	Rh(1)-Rh(2)-Rh(4)	59.30(3)
U(2)-Rh(2)-Rh(4)	60.70(3)	P(5)-Rh(2)-U(1)	146.41(9)
P(1)-Rh(2)-U(1)	72.06(8)	Rh(1)-Rh(2)-U(1)	46.57(2)
U(2)-Rh(2)-U(1)	119.25(4)	Rh(4)-Rh(2)-U(1)	58.55(3)
P(5)-Rh(2)-Rh(3)	109.92(8)	P(1)-Rh(2)-Rh(3)	103.76(9)

Rh(1)-Rh(2)-Rh(3)	115.14(5)	U(2)-Rh(2)-Rh(3)	45.50(3)
Rh(4)-Rh(2)-Rh(3)	55.85(3)	U(1)-Rh(2)-Rh(3)	97.04(4)
P(4)-Rh(3)-U(2)	83.84(8)	P(4)-Rh(3)-Rh(4)	143.21(9)
U(2)-Rh(3)-Rh(4)	70.49(3)	P(4)-Rh(3)-Rh(2)	131.03(9)
U(2)-Rh(3)-Rh(2)	65.26(3)	Rh(4)-Rh(3)-Rh(2)	60.62(4)
P(2)-Rh(4)-P(6)	115.72(12)	P(2)-Rh(4)-Rh(3)	97.35(9)
P(6)-Rh(4)-Rh(3)	108.24(8)	P(2)-Rh(4)-Rh(1)	113.77(9)
P(6)-Rh(4)-Rh(1)	99.98(8)	Rh(3)-Rh(4)-Rh(1)	122.67(5)
P(2)-Rh(4)-U(1)	75.15(8)	P(6)-Rh(4)-U(1)	143.59(9)
Rh(3)-Rh(4)-U(1)	104.24(4)	Rh(1)-Rh(4)-U(1)	47.22(2)
P(2)-Rh(4)-Rh(2)	123.07(9)	P(6)-Rh(4)-Rh(2)	121.16(9)
Rh(3)-Rh(4)-Rh(2)	63.53(4)	Rh(1)-Rh(4)-Rh(2)	59.15(3)
U(1)-Rh(4)-Rh(2)	61.12(3)	P(2)-Rh(4)-U(2)	141.91(9)
P(6)-Rh(4)-U(2)	73.58(8)	Rh(3)-Rh(4)-U(2)	47.03(3)
Rh(1)-Rh(4)-U(2)	99.58(4)	U(1)-Rh(4)-U(2)	120.66(4)
Rh(2)-Rh(4)-U(2)	59.54(3)	C(8)-N(6)-P(4)	128.2(8)
C(8)-N(6)-U(2)	129.1(7)	P(4)-N(6)-U(2)	100.8(5)
C(10)-N(7)-P(5)	127.2(8)	C(10)-N(7)-U(2)	128.9(7)
P(5)-N(7)-U(2)	103.7(4)	C(12)-N(8)-P(6)	125.4(8)
C(12)-N(8)-U(2)	125.5(7)	P(6)-N(8)-U(2)	107.7(5)
C(7)-N(5)-C(11)	111.7(9)	C(7)-N(5)-C(9)	111.3(9)
C(11)-N(5)-C(9)	109.9(9)	C(7)-N(5)-U(2)	109.2(7)
C(11)-N(5)-U(2)	106.7(6)	C(9)-N(5)-U(2)	107.8(7)
N(6)-P(4)-C(31)	109.1(6)	N(6)-P(4)-C(34)	106.0(5)
C(31)-P(4)-C(34)	103.5(6)	N(6)-P(4)-Rh(3)	95.3(4)
C(31)-P(4)-Rh(3)	119.2(4)	C(34)-P(4)-Rh(3)	122.3(4)
N(6)-P(4)-U(2)	47.2(3)	C(31)-P(4)-U(2)	130.1(4)
C(34)-P(4)-U(2)	123.9(4)	Rh(3)-P(4)-U(2)	48.25(6)
N(7)-P(5)-C(40)	103.8(5)	N(7)-P(5)-C(37)	106.0(5)
C(40)-P(5)-C(37)	102.1(5)	N(7)-P(5)-Rh(2)	106.9(4)
C(40)-P(5)-Rh(2)	121.4(4)	C(37)-P(5)-Rh(2)	115.2(4)
N(7)-P(5)-U(2)	44.6(3)	C(40)-P(5)-U(2)	135.1(4)
C(37)-P(5)-U(2)	115.8(4)	Rh(2)-P(5)-U(2)	63.38(8)
N(8)-P(6)-C(43)	104.1(5)	N(8)-P(6)-C(46)	108.6(5)
C(43)-P(6)-C(46)	100.0(5)	N(8)-P(6)-Rh(4)	104.8(4)
C(43)-P(6)-Rh(4)	121.4(4)	C(46)-P(6)-Rh(4)	116.9(4)
N(8)-P(6)-U(2)	43.0(3)	C(43)-P(6)-U(2)	120.5(4)
C(46)-P(6)-U(2)	133.1(4)	Rh(4)-P(6)-U(2)	62.30(7)
N(5)-C(7)-C(8)	111.6(9)	N(6)-C(8)-C(7)	106.1(9)
N(5)-C(9)-C(10)	109.2(9)	N(7)-C(10)-C(9)	107.5(9)
(5)-C(11)-C(12)	112.7(9)	N(8)-C(12)-C(11)	109.0(9)
N(2)-P(2)-C(22)	110.7(6)	N(2)-P(2)-C(19)	102.7(5)
C(22)-P(2)-C(19)	98.8(5)	N(2)-P(2)-Rh(4)	103.7(4)

C(22)-P(2)-Rh(4)	117.7(4)	C(19)-P(2)-Rh(4)	122.3(4)
N(2)-P(2)-U(1)	43.3(4)	C(22)-P(2)-U(1)	132.9(4)
C(19)-P(2)-U(1)	122.3(4)	Rh(4)-P(2)-U(1)	60.55(8)
N(4)-P(1)-C(16)	108.4(6)	N(4)-P(1)-C(13)	103.7(6)
C(16)-P(1)-C(13)	100.5(5)	N(4)-P(1)-Rh(2)	105.4(4)
C(16)-P(1)-Rh(2)	114.8(4)	C(13)-P(1)-Rh(2)	123.0(4)
N(4)-P(1)-U(1)	43.9(4)	C(16)-P(1)-U(1)	136.0(4)
C(13)-P(1)-U(1)	117.4(4)	Rh(2)-P(1)-U(1)	62.98(8)
C(2)-N(4)-P(1)	125.6(11)	C(2)-N(4)-U(1)	126.9(9)
P(1)-N(4)-U(1)	104.9(5)	N(1)-C(1)-C(2)	110.8(10)
N(4)-C(2)-C(1)	109.4(10)	C(4)-N(2)-P(2)	125.9(10)
C(4)-N(2)-U(1)	126.3(10)	P(2)-N(2)-U(1)	107.4(5)
N(1)-C(3)-C(4)	111.4(10)	N(2)-C(4)-C(3)	108.0(11)
N(1)-C(5)-C(6)	114.9(10)	N(3)-C(6)-C(5)	104.9(9)
C(14)-C(13)-C(15)	110.5(10)	C(14)-C(13)-P(1)	111.4(9)
C(15)-C(13)-P(1)	112.4(9)	C(18)-C(16)-C(17)	108.1(10)
C(18)-C(16)-P(1)	118.0(9)	C(17)-C(16)-P(1)	111.7(8)
C(21)-C(19)-C(20)	109.3(9)	C(21)-C(19)-P(2)	112.1(8)
C(20)-C(19)-P(2)	113.1(8)	C(24)-C(22)-C(23)	109.0(9)
C(24)-C(22)-P(2)	108.1(8)	C(23)-C(22)-P(2)	118.8(9)
C(33)-C(31)-C(32)	109.7(10)	C(33)-C(31)-P(4)	117.8(9)
C(32)-C(31)-P(4)	112.6(9)	C(36)-C(34)-C(35)	108.5(10)
C(36)-C(34)-P(4)	113.2(9)	C(35)-C(34)-P(4)	110.5(8)
C(39)-C(37)-C(38)	109.9(9)	C(39)-C(37)-P(5)	117.5(8)
C(38)-C(37)-P(5)	107.8(8)	C(42)-C(40)-C(41)	109.6(9)
C(42)-C(40)-P(5)	111.5(8)	C(41)-C(40)-P(5)	111.3(9)
C(45)-C(43)-C(44)	108.9(9)	C(45)-C(43)-P(6)	111.9(9)
C(44)-C(43)-P(6)	112.0(8)	C(48)-C(46)-C(47)	109.5(9)
C(48)-C(46)-P(6)	108.6(8)	C(47)-C(46)-P(6)	119.4(8)
N(6')-U(2')-Rh(3')	82.1(16)	N(6')-U(2')-N(7')	107(3)
Rh(3')-U(2')-N(7')	119.1(15)	N(6')-U(2')-N(8')	100(3)
Rh(3')-U(2')-N(8')	132.1(15)	N(7')-U(2')-N(8')	106(2)
N(6')-U(2')-N(5')	65(2)	Rh(3')-U(2')-N(5')	145.3(12)
N(7')-U(2')-N(5')	65.2(19)	N(8')-U(2')-N(5')	67.4(19)
N(6')-U(2')-Rh(4')	127.8(18)	Rh(3')-U(2')-Rh(4')	65.6(3)
N(7')-U(2')-Rh(4')	124.0(16)	N(8')-U(2')-Rh(4')	77.1(15)
N(5')-U(2')-Rh(4')	144.3(12)	N(6')-U(2')-Rh(2')	136.5(18)
Rh(3')-U(2')-Rh(2')	61.9(3)	N(7')-U(2')-Rh(2')	74.2(15)
N(8')-U(2')-Rh(2')	122.3(16)	N(5')-U(2')-Rh(2')	139.1(12)
Rh(4')-U(2')-Rh(2')	59.7(2)	N(6')-U(2')-P(4')	33.1(17)
Rh(3')-U(2')-P(4')	49.1(5)	N(7')-U(2')-P(4')	117.0(18)
N(8')-U(2')-P(4')	121.9(17)	N(5')-U(2')-P(4')	96.9(12)
Rh(4')-U(2')-P(4')	105.5(5)	Rh(2')-U(2')-P(4')	106.1(5)

N(6')-U(2')-P(6')	113(2)	Rh(3')-U(2')-P(6')	104.6(5)
N(7')-U(2')-P(6')	123.3(18)	N(8')-U(2')-P(6')	30.9(15)
N(5')-U(2')-P(6')	98.3(12)	Rh(4')-U(2')-P(6')	46.4(5)
Rh(2')-U(2')-P(6')	99.5(5)	P(4')-U(2')-P(6')	118.7(6)
N(6')-U(2')-P(5')	127(2)	Rh(3')-U(2')-P(5')	98.1(4)
N(7')-U(2')-P(5')	29.0(15)	N(8')-U(2')-P(5')	116.7(17)
N(5')-U(2')-P(5')	93.9(12)	Rh(4')-U(2')-P(5')	98.3(5)
Rh(2')-U(2')-P(5')	45.3(4)	P(4')-U(2')-P(5')	120.1(6)
P(6')-U(2')-P(5')	117.5(6)	P(1')-Rh(2')-P(5')	117.3(9)
P(1')-Rh(2')-Rh(3')	100.7(7)	P(5')-Rh(2')-Rh(3')	107.5(7)
P(1')-Rh(2')-U(1)	72.0(7)	P(5')-Rh(2')-U(1)	146.2(6)
Rh(3')-Rh(2')-U(1)	101.9(3)	P(1')-Rh(2')-Rh(4')	123.0(7)
P(5')-Rh(2')-Rh(4')	119.7(6)	Rh(3')-Rh(2')-Rh(4')	60.4(3)
U(1)-Rh(2')-Rh(4')	62.4(3)	P(1')-Rh(2')-Rh(1)	111.1(8)
P(5')-Rh(2')-Rh(1)	104.2(6)	Rh(3')-Rh(2')-Rh(1)	116.7(3)
U(1)-Rh(2')-Rh(1)	46.15(14)	Rh(4')-Rh(2')-Rh(1)	56.3(2)
P(1')-Rh(2')-U(2')	144.8(7)	P(5')-Rh(2')-U(2')	71.0(6)
Rh(3')-Rh(2')-U(2')	47.0(2)	U(1)-Rh(2')-U(2')	121.6(3)
Rh(4')-Rh(2')-U(2')	59.2(3)	Rh(1)-Rh(2')-U(2')	98.3(3)
P(4')-Rh(3')-U(2')	81.6(6)	P(4')-Rh(3')-Rh(2')	140.6(7)
U(2')-Rh(3')-Rh(2')	71.1(3)	P(4')-Rh(3')-Rh(4')	131.2(7)
U(2')-Rh(3')-Rh(4')	67.6(3)	Rh(2')-Rh(3')-Rh(4')	62.5(3)
P(2')-Rh(4')-P(6')	121.2(9)	P(2')-Rh(4')-Rh(1)	104.0(7)
P(6')-Rh(4')-Rh(1)	102.3(6)	P(2')-Rh(4')-Rh(3')	102.6(7)
P(6')-Rh(4')-Rh(3')	108.2(7)	Rh(1)-Rh(4')-Rh(3')	119.6(3)
P(2')-Rh(4')-U(2')	146.5(7)	P(6')-Rh(4')-U(2')	69.3(6)
Rh(1)-Rh(4')-U(2')	104.1(3)	Rh(3')-Rh(4')-U(2')	46.8(2)
P(2')-Rh(4')-Rh(2')	118.7(8)	P(6')-Rh(4')-Rh(2')	120.1(7)
Rh(1)-Rh(4')-Rh(2')	62.6(2)	Rh(3')-Rh(4')-Rh(2')	57.1(3)
U(2')-Rh(4')-Rh(2')	61.1(3)	P(2')-Rh(4')-U(1)	70.8(7)
P(6')-Rh(4')-U(1)	147.9(6)	Rh(1)-Rh(4')-U(1)	46.40(14)
Rh(3')-Rh(4')-U(1)	96.3(3)	U(2')-Rh(4')-U(1)	118.7(3)
Rh(2')-Rh(4')-U(1)	57.6(2)	N(7')-P(5')-C(37')	110(4)
N(7')-P(5')-C(40')	97(3)	C(37')-P(5')-C(40')	100(3)
N(7')-P(5')-Rh(2')	109(2)	C(37')-P(5')-Rh(2')	118(2)
C(40')-P(5')-Rh(2'	120(2)	N(7')-P(5')-U(2')	46(2)
C(37')-P(5')-U(2')	136.5(18)	C(40')-P(5')-U(2')	116.5(18)
Rh(2')-P(5')-U(2')	63.7(5)	C(7')-N(5')-C(11')	113(6)
C(7')-N(5')-C(9')	112(6)	C(11')-N(5')-C(9')	108(5)
C(7')-N(5')-U(2')	104(4)	C(11')-N(5')-U(2')	105(4)
C(9')-N(5')-U(2')	115(4)	N(5')-C(9')-C(10')	106(5)
N(7')-C(10')-C(9')	116(6)	C(10')-N(7')-P(5')	130(5)
C(10')-N(7')-U(2')	124(5)	P(5')-N(7')-U(2')	105(3)

N(5')-C(7')-C(8')	116(6)	N(6')-C(8')-C(7')	97(6)
C(8')-N(6')-P(4')	124(5)	C(8')-N(6')-U(2')	132(5)
P(4')-N(6')-U(2')	99(3)	N(6')-P(4')-C(31')	99(3)
N(6')-P(4')-C(34')	113(4)	C(31')-P(4')-C(34')	116(3)
N(6')-P(4')-Rh(3')	97(2)	C(31')-P(4')-Rh(3')	116.0(18)
C(34')-P(4')-Rh(3')	113(2)	N(6')-P(4')-C(32')	139(3)
C(31')-P(4')-C(32')	40.9(14)	C(34')-P(4')-C(32')	86(3)
Rh(3')-P(4')-C(32')	109.0(18)	N(6')-P(4')-U(2')	48(2)
C(31')-P(4')-U(2')	113.5(19)	C(34')-P(4')-U(2')	130(3)
Rh(3')-P(4')-U(2')	49.3(5)	C(32')-P(4')-U(2')	142.0(14)
N(8')-P(6')-C(46')	103(4)	N(8')-P(6')-C(43')	100(3)
C(46')-P(6')-C(43')	103(3)	N(8')-P(6')-Rh(4')	114(3)
C(46')-P(6')-Rh(4')	112(2)	C(43')-P(6')-Rh(4')	122(2)
N(8')-P(6')-U(2')	51(2)	C(46')-P(6')-U(2')	116(2)
C(43')-P(6')-U(2')	135(2)	Rh(4')-P(6')-U(2')	64.2(6)
C(12')-N(8')-P(6')	138(6)	C(12')-N(8')-U(2')	124(5)
P(6')-N(8')-U(2')	98(3)	N(8')-C(12')-C(11')	108(6)
N(5')-C(11')-C(12')	114(6)	C(14')-C(13')-C(15')	107.4(19)
C(14')-C(13')-P(1')	116(5)	C(15')-C(13')-P(1')	118(6)
C(18')-C(16')-C(17')	114(6)	C(18')-C(16')-P(1')	108(4)
C(17')-C(16')-P(1')	120(5)	C(21')-C(19')-C(20')	108.1(19)
C(21')-C(19')-P(2')	114(5)	C(20')-C(19')-P(2')	113(5)
C(23')-C(22')-C(24')	106.9(17)	C(23')-C(22')-P(2')	118(6)
C(24')-C(22')-P(2')	115(5)	C(19')-P(2')-C(22')	93(3)
C(19')-P(2')-N(2')	119(3)	C(22')-P(2')-N(2')	92(3)
C(19')-P(2')-Rh(4')	116(2)	C(22')-P(2')-Rh(4')	124(3)
N(2')-P(2')-Rh(4')	110(3)	C(19')-P(2')-U(1)	137(2)
C(22')-P(2')-U(1)	124(2)	N(2')-P(2')-U(1)	46(3)
Rh(4')-P(2')-U(1)	64.5(7)	N(4')-P(1')-C(16')	98(4)
N(4')-P(1')-C(13')	112(5)	C(16')-P(1')-C(13')	102(3)
N(4')-P(1')-C(2')	36(3)	C(16')-P(1')-C(2')	65(3)
C(13')-P(1')-C(2')	105(3)	N(4')-P(1')-Rh(2')	104(4)
C(16')-P(1')-Rh(2')	120(3)	C(13')-P(1')-Rh(2')	119(2)
C(2')-P(1')-Rh(2')	131(2)	N(4')-P(1')-U(1)	42(4)
C(16')-P(1')-U(1)	115.6(19)	C(13')-P(1')-U(1)	135(3)
C(2')-P(1')-U(1)	72(2)	Rh(2')-P(1')-U(1)	61.9(6)
P(1')-N(4')-C(2')	111(7)	P(1')-N(4')-U(1)	115(4)
C(2')-N(4')-U(1)	121(7)	N(1)-C(1')-C(2')	108(5)
N(4')-C(2')-C(1')	115(7)	N(4')-C(2')-P(1')	33(4)
C(1')-C(2')-P(1')	147(5)	N(1)-C(3')-C(4')	120(5)
N(2')-C(4')-C(3')	104(7)	C(4')-N(2')-P(2')	132(6)
C(4')-N(2')-U(1)	131(7)	P(2')-N(2')-U(1)	93(3)
N(1)-C(5')-C(6')	95(5)	N(3)-C(6')-C(5')	105(4)

C(33')-C(31')-C(32')	107.9(19)	C(33')-C(31')-P(4')	118(2)
C(32')-C(31')-P(4')	88(3)	C(31')-C(32')-P(4')	51(2)
C(36')-C(34')-C(35')	107.1(19)	C(36')-C(34')-P(4')	139(5)
C(35')-C(34')-P(4')	106(4)	C(38')-C(37')-C(39')	108.1(19)
C(38')-C(37')-P(5')	110(4)	C(39')-C(37')-P(5')	121(5)
C(42')-C(40')-C(41')	119(2)	C(42')-C(40')-P(5')	105(4)
C(41')-C(40')-P(5')	117(5)	C(45')-C(43')-C(44')	107.7(19)
C(45')-C(43')-P(6')	109(5)	C(44')-C(43')-P(6')	109(5)
C(48')-C(46')-C(47')	106.9(19)	C(48')-C(46')-P(6')	120(5)
C(47')-C(46')-P(6')	118(4)	P(3)-Rh(1)-U(1)	84.52(7)
P(3)-Rh(1)-Rh(4')	146.9(2)	U(1)-Rh(1)-Rh(4')	71.77(17)
P(3)-Rh(1)-Rh(2)	138.66(8)	U(1)-Rh(1)-Rh(2)	68.82(3)
P(3)-Rh(1)-Rh(4)	135.38(8)	U(1)-Rh(1)-Rh(4)	66.65(3)
Rh(2)-Rh(1)-Rh(4)	61.55(4)	P(3)-Rh(1)-Rh(2')	128.23(19)
U(1)-Rh(1)-Rh(2')	64.34(17)	Rh(4')-Rh(1)-Rh(2')	61.1(2)
N(3)-P(3)-C(25)	107.8(5)	N(3)-P(3)-C(28)	110.6(5)
C(25)-P(3)-C(28)	100.6(5)	N(3)-P(3)-Rh(1)	94.8(3)
C(25)-P(3)-Rh(1)	120.7(4)	C(28)-P(3)-Rh(1)	121.6(4)
N(3)-P(3)-U(1)	47.2(3)	C(25)-P(3)-U(1)	122.2(4)
C(28)-P(3)-U(1)	135.2(4)	Rh(1)-P(3)-U(1)	48.03(6)
C(6)-N(3)-P(3)	128.5(8)	C(6')-N(3)-P(3)	135(2)
C(6)-N(3)-U(1)	129.4(7)	C(6')-N(3)-U(1)	114(4)
P(3)-N(3)-U(1)	101.3(4)	C(5')-N(1)-C(1')	118(4)
C(5')-N(1)-C(3')	110(4)	C(1')-N(1)-C(3')	105(5)
C(5)-N(1)-C(3)	114.0(9)	C(5)-N(1)-C(1)	108.3(9)
C(3)-N(1)-C(1)	111.8(9)	C(5')-N(1)-U(1)	108(3)
C(1')-N(1)-U(1)	110(3)	C(5)-N(1)-U(1)	107.5(7)
C(3')-N(1)-U(1)	106(3)	C(3)-N(1)-U(1)	108.2(7)
C(1)-N(1)-U(1)	106.8(6)	C(27)-C(25)-C(26)	111.5(10)
C(27)-C(25)-P(3)	111.5(9)	C(26)-C(25)-P(3)	108.0(8)
C(30)-C(28)-C(29)	111.2(11)	C(30)-C(28)-P(3)	111.8(9)
C(29)-C(28)-P(3)	114.3(9)	C(50)-C(49)-C(54)	124.1(17)
C(49)-C(50)-C(51)	117.5(16)	C(50)-C(51)-C(52)	120.8(17)
C(53)-C(52)-C(51)	117.8(16)	C(53)-C(52)-C(55)	121.6(15)
C(51)-C(52)-C(55)	120.5(16)	C(54)-C(53)-C(52)	123.1(16)
C(53)-C(54)-C(49)	116.7(17)		

4. Computational Methods

The Gaussian09 program suite was used for all quantum-chemical calculations (4). We used Becke's 3-parameter hybrid version (5), combined with the non-local correlation functional provided by Perdew/Wang (6), denoted as B3PW91. The relativistic energy-consistent small-core pseudopotential of the Stuttgart-Köln ECP library was used in combination with its adapted segmented basis set to represent a uranium atom (7-9). In specific cases, the *f*-in-core RECPs adapted to either a U(III) or U(IV) core configuration (either $5f^3$ or $5f^2$) were used in association with the adapted basis set. For phosphorus, chlorine and rhodium, the quasi-relativistic energy-adjusted *ab-initio* pseudopotentials were used, along with their corresponding energy-optimized valence basis sets (10, 11). For all the atoms, the 6-31G(d) basis set was used (12,13). In all computations no constraints were imposed on the geometry. A full geometry optimization was performed for each structure using Schlegel's analytical gradient method (14) and the attainment of the energy minimum was verified by calculating the vibrational frequencies that result in the absence of imaginary eigenvalues. All stationary points have been identified for the minimum (number of imaginary frequencies, Nimag = 0). The NBO analysis (15) was carried out on the optimized structures using the module included in the Gaussian package. Finally, the Chemcraft graphical program was used for the 3D representations of the structures and the orbital plots (16). Complete Active Space Calculations (CASSCF) were carried out using the Gaussian package.

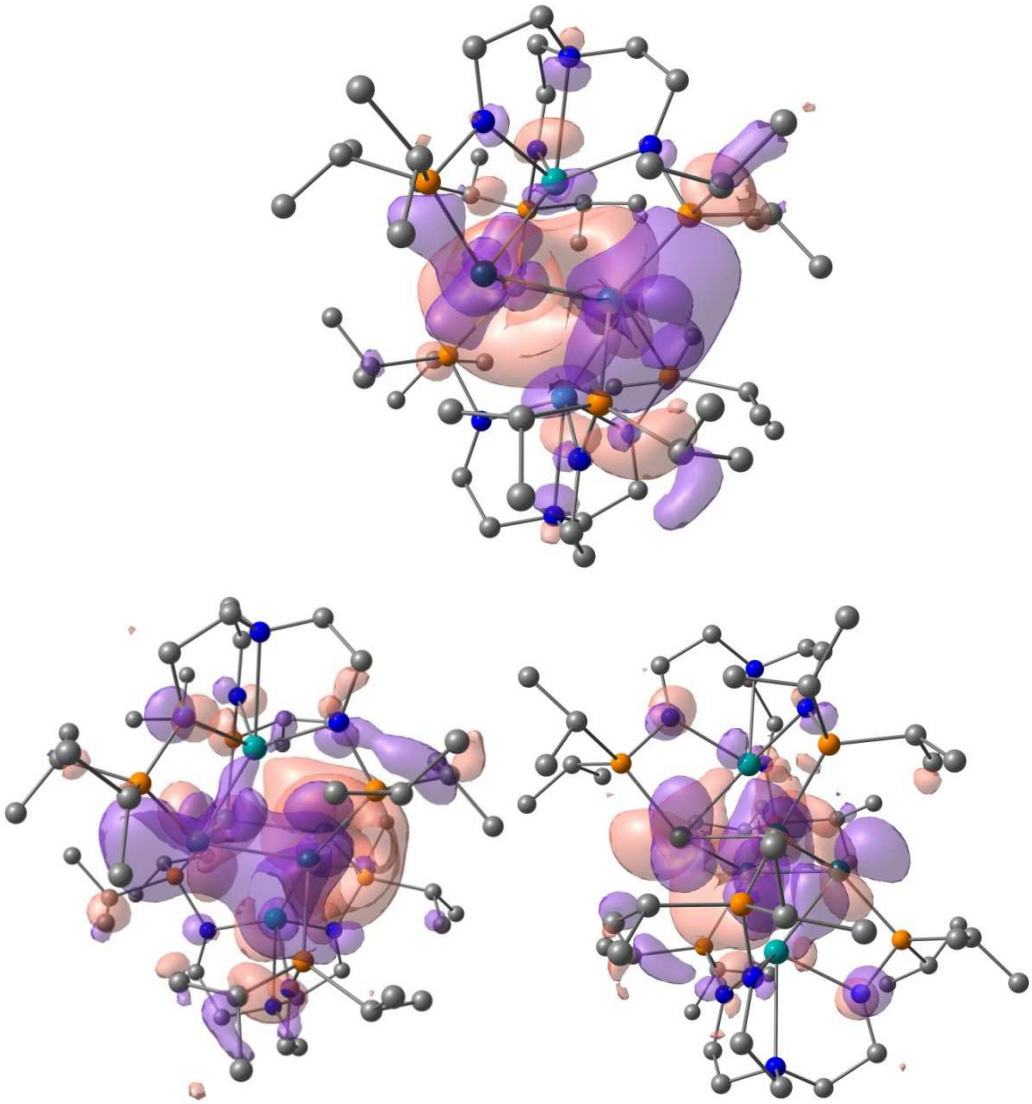

Fig. S10. Bonding U-Rh molecular orbitals of complex **3**. The first one is a σ orbital while the two others are π-type orbitals.

Optimized structure of complex **3**

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U	2.136664	10.758474	7.203112
U	3.837883	10.239925	2.413351
Rh	5.368247	10.342523	4.142722
Rh	3.016495	11.913622	4.626383
Rh	2.975633	8.988277	4.972942
Rh	0.607272	10.813229	5.477168
P	2.213000	12.970508	2.727540
P	2.272142	7.600691	3.202060
P	3.814912	13.341869	6.296344
P	-0.932948	10.871102	7.184451
P	3.639279	8.031686	6.981085
P	6.924154	10.185305	2.459813

N	2.552472	8.491142	1.793733
N	3.188602	12.714351	7.673824
N	2.458769	11.108285	9.802691
N	3.536750	10.036219	-0.201843
N	2.802459	12.050239	1.470023
N	3.365087	9.152543	8.195568
N	0.179048	10.655604	8.420260
N	5.863613	9.996914	1.287222
C	5.644472	13.470625	6.649378
H	5.759444	14.080523	7.407239
C	1.296817	10.472635	10.522469
H	1.280045	10.776229	11.444090
H	1.403105	9.508995	10.522469
C	6.219206	12.074635	7.072105
H	7.159707	12.155955	7.247289
H	6.077008	11.443051	6.363752
H	5.771397	11.772396	7.868050
C	6.353203	8.609056	7.110188
H	7.251939	8.302752	7.243480
H	6.136084	9.266391	7.776649
H	6.275827	9.002102	6.238076
C	0.392637	13.107396	2.361177
H	0.305141	13.539747	1.485256
C	2.653394	6.494741	7.487215
H	2.720037	5.836051	6.763628
C	-1.908112	12.414823	7.609082
H	-2.366846	12.272513	8.462152
C	3.373313	15.175630	6.158101
H	3.613715	15.442630	5.244097
C	3.720742	10.449594	10.202568
H	3.766351	10.385894	11.169888
H	4.476659	10.976818	9.897900
C	7.966415	11.651772	2.007000
H	8.473096	11.420011	1.199630
C	-0.027874	10.848061	9.829349
H	-0.748185	10.281533	10.145442
H	-0.255988	11.772396	10.012150
C	2.248900	8.080477	0.437960
H	2.194013	7.112772	0.396068
H	1.387961	8.442351	0.175184
C	5.406253	7.450249	7.224439
H	5.474219	7.110061	8.138442
C	4.208917	14.827310	2.330710
H	4.485534	15.732671	2.201226

H	4.490785	14.293310	1.580465
H	4.606720	14.478990	3.134271
C	3.414577	13.241574	9.018171
H	3.235361	14.194371	9.025788
H	4.342639	13.106041	9.265714
C	3.783351	9.046828	9.585615
H	4.687787	8.699863	9.635124
H	3.196361	8.443706	10.065467
C	2.690782	14.764965	2.448769
H	2.449720	15.252884	3.263755
C	-0.253046	11.701919	2.243118
H	-1.182823	11.794082	2.026042
H	-0.164012	11.238396	3.077146
H	0.189796	11.204513	1.549998
C	2.505436	12.538158	10.019767
H	2.824233	12.714351	10.918537
H	1.608898	12.900031	9.943600
C	8.246637	8.855726	2.448769
H	8.815807	9.050894	3.218055
C	0.468451	7.114127	3.301839
H	0.329669	6.741411	4.196801
C	3.103608	5.978361	2.810562
H	2.672244	5.602934	2.014617
C	4.059124	16.183996	7.087338
H	3.738183	17.067671	6.896921
H	5.011347	16.152823	6.946429
H	3.864649	15.964432	8.001342
C	-0.366334	13.943635	3.343731
H	-1.287255	13.996493	3.077146
H	0.008553	14.825955	3.374197
H	-0.308640	13.543813	4.215843
C	4.540935	6.165396	2.502085
H	4.934411	5.315604	2.292626
H	4.982266	6.544889	3.263755
H	4.631222	6.754965	1.751841
C	7.048569	12.832264	1.656632
H	7.582498	13.585828	1.393856
H	6.522052	13.066737	2.425918
H	6.468297	12.584239	0.933046
C	2.053009	15.532082	1.260564
H	2.377323	16.430666	1.245330
H	1.097075	15.533437	1.359581
H	2.284329	15.090244	0.437960
C	6.032176	9.799036	-0.198034

H	6.086549	8.854371	-0.415110
H	6.831597	10.243584	-0.517936
C	5.775251	6.330746	6.310435
H	6.682391	6.066457	6.478002
H	5.687224	6.618076	5.400239
H	5.191555	5.583960	6.466577
C	3.116169	5.830630	8.785862
H	2.562629	5.067579	8.968663
H	3.042965	6.458147	9.509448
H	4.029356	5.551432	8.694461
C	2.519577	12.233209	0.038083
H	3.230042	12.744168	-0.377027
H	1.685871	12.715706	-0.076167
C	6.413909	14.031731	5.495448
H	7.343106	14.095432	5.731566
H	6.078179	14.905919	5.282180
H	6.313750	13.455716	4.733778
C	-2.186056	9.487310	7.342497
H	-1.645551	8.682244	7.475790
C	0.019642	6.031219	2.311668
H	-0.911384	5.850960	2.437344
H	0.531456	5.235640	2.456385
H	0.166676	6.347010	1.412898
C	-2.966264	12.712995	6.531319
H	-3.437739	13.523483	6.759820
H	-3.586886	11.987894	6.478002
H	-2.533775	12.833620	5.678249
C	-0.993831	13.580407	7.757607
H	-1.503915	14.366498	7.978492
H	-0.524624	13.730848	6.931196
H	-0.360113	13.405569	8.458344
C	2.421744	10.856193	-0.601719
H	1.590500	10.438752	-0.331326
H	2.412498	10.955132	-1.565232
C	1.185702	6.952843	7.586232
H	0.629867	6.210122	7.818541
H	0.903976	7.312005	6.736970
H	1.108231	7.637285	8.260310
C	8.931804	12.008224	3.054296
H	9.458263	12.756366	2.761053
H	9.507891	11.260082	3.225672
H	8.461309	12.244051	3.854049
C	-0.427684	8.308173	3.195205
H	-1.343850	8.030330	3.263755

H	-0.288572	8.740523	2.349751
H	-0.226437	8.924848	3.903558
C	1.855202	15.305742	6.249501
H	1.609692	16.231432	6.184759
H	1.552822	14.949290	7.087338
H	1.449453	14.817823	5.525915
C	3.289566	8.552132	-0.487469
H	2.998905	8.435574	-1.405281
H	4.106946	8.050660	-0.354176
C	4.771331	10.436041	-0.807370
H	4.850192	11.395615	-0.742628
H	4.738820	10.202924	-1.748032
C	9.164754	8.835396	1.264372
H	9.784217	8.110295	1.355772
H	9.640753	9.664858	1.214863
H	8.647541	8.716127	0.460810
C	2.909068	4.951020	4.002575
H	3.322428	4.116137	3.777882
H	1.967898	4.811421	4.151101
H	3.307628	5.306117	4.798520
C	-3.124742	9.500863	8.469769
H	-3.714982	8.743234	8.401218
H	-3.648285	10.308640	8.443110
H	-2.643916	9.458848	9.296181
C	7.669026	7.576295	2.715353
H	8.366183	6.909472	2.711545
H	7.023475	7.366219	2.041275
H	7.247589	7.588493	3.576040
C	-2.912607	9.243351	6.070509
H	-3.539203	8.530447	6.196184
H	-2.284190	9.007523	5.385006
H	-3.380643	10.042995	5.815349

Optimized structure of complex **3** assuming $5f^2$ configuration (U^{IV})
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U	2.139555	10.757243	7.210396
U	3.830038	10.237180	2.401299
Rh	5.377346	10.341345	4.166730
Rh	3.013021	11.918396	4.623243
Rh	2.977658	8.976900	4.974237
Rh	0.589688	10.808271	5.448185
P	2.194534	12.980999	2.726612
P	2.260366	7.579359	3.202557

P	3.826493	13.356584	6.288869
P	-0.953251	10.873359	7.167382
P	3.653137	8.013273	6.982098
P	6.946134	10.189172	2.480651
N	2.535126	8.473767	1.784081
N	3.195614	12.725954	7.686217
N	2.463025	11.109215	9.815143
N	3.526773	10.033612	-0.219849
N	2.786575	12.057416	1.454543
N	3.377746	9.139857	8.208803
N	0.171898	10.657014	8.423428
N	5.862904	9.995818	1.271137
C	5.664859	13.490078	6.632801
H	5.785838	14.134017	7.426145
C	1.301638	10.478941	10.533170
H	1.287209	10.801674	11.506983
H	1.413534	9.462768	10.531927
C	6.245043	12.105286	7.056430
H	7.243954	12.199161	7.235347
H	6.093376	11.431130	6.307468
H	5.778131	11.784005	7.903326
C	6.383981	8.594143	7.108483
H	7.337933	8.264692	7.247792
H	6.160215	9.292108	7.815766
H	6.304534	9.016646	6.183641
C	0.363352	13.115480	2.372346
H	0.265671	13.571310	1.454627
C	2.664201	6.468170	7.478653
H	2.736973	5.784536	6.713513
C	-1.928133	12.424940	7.593545
H	-2.409204	12.275606	8.490540
C	3.384295	15.194374	6.143312
H	3.633894	15.467539	5.182184
C	3.725977	10.447326	10.215889
H	3.773221	10.381710	11.238761
H	4.521431	11.003830	9.892266
C	7.996632	11.666491	2.034120
H	8.531291	11.424542	1.187969
C	-0.027729	10.853090	9.842335
H	-0.785011	10.254600	10.185138
H	-0.265601	11.830493	10.039470
C	2.226524	8.061936	0.424518
H	2.173179	7.039663	0.372130
H	1.315087	8.439760	0.147070

C	5.425724	7.428824	7.221245
H	5.495341	7.068050	8.181540
C	4.198005	14.852227	2.328555
H	4.487667	15.817705	2.192715
H	4.497528	14.291361	1.531186
H	4.627634	14.482265	3.175399
C	3.423795	13.257137	9.031888
H	3.231718	14.262562	9.044192
H	4.404274	13.115639	9.295701
C	3.794506	9.039348	9.603037
H	4.751348	8.677952	9.661620
H	3.175592	8.404128	10.114457
C	2.674213	14.782883	2.454115
H	2.423540	15.290209	3.313437
C	-0.279829	11.712002	2.255289
H	-1.269185	11.810979	2.033125
H	-0.177541	11.217714	3.140408
H	0.182658	11.184232	1.516809
C	2.510989	12.550174	10.034761
H	2.847687	12.738923	10.985427
H	1.564749	12.930481	9.952521
C	8.273527	8.852978	2.473719
H	8.867690	9.060423	3.286998
C	0.451260	7.088384	3.306026
H	0.309948	6.698941	4.247847
C	3.092690	5.947233	2.815330
H	2.635146	5.551092	1.983227
C	4.083009	16.201679	7.071735
H	3.744883	17.140383	6.867160
H	5.091083	16.166537	6.921405
H	3.881748	15.975877	8.044184
C	-0.393440	13.956111	3.374533
H	-1.373504	14.012717	3.100876
H	0.000152	14.894817	3.410778
H	-0.324951	13.529536	4.298132
C	4.545924	6.135364	2.499790
H	4.964089	5.232627	2.279265
H	5.020153	6.541085	3.303450
H	4.644867	6.758409	1.701377
C	7.083422	12.852319	1.682356
H	7.654909	13.651343	1.409789
H	6.521286	13.099664	2.495299
H	6.469905	12.596964	0.910950
C	2.024832	15.545535	1.270275

H	2.367472	16.502544	1.255771
H	1.011513	15.545694	1.376609
H	2.266461	15.081711	0.395024
C	6.030698	9.801810	-0.205692
H	6.088863	8.804743	-0.433226
H	6.874694	10.273591	-0.541724
C	5.793842	6.301234	6.291149
H	6.756700	6.017232	6.465708
H	5.700850	6.609648	5.325602
H	5.175985	5.506233	6.449499
C	3.131129	5.795835	8.776747
H	2.545761	4.982790	8.963509
H	3.051371	6.452495	9.550721
H	4.101159	5.501350	8.682821
C	2.500517	12.242309	0.022941
H	3.250329	12.783848	-0.416100
H	1.618669	12.748725	-0.099655
C	6.432162	14.052612	5.460068
H	7.419688	14.124788	5.702663
H	6.075930	14.978391	5.226083
H	6.323555	13.436776	4.655652
C	-2.213590	9.487140	7.327389
H	-1.643468	8.642297	7.468888
C	0.001691	5.999058	2.314186
H	-0.987922	5.807655	2.451126
H	0.542943	5.151498	2.464513
H	0.152976	6.328425	1.360150
C	-2.989932	12.726772	6.517014
H	-3.484837	13.586368	6.761482
H	-3.655144	11.960875	6.458293
H	-2.533864	12.853260	5.612615
C	-0.997895	13.598341	7.741638
H	-1.534431	14.434149	7.976893
H	-0.500604	13.756868	6.865742
H	-0.322619	13.414648	8.482185
C	2.403043	10.860605	-0.622892
H	1.527159	10.418677	-0.336367
H	2.391803	10.966967	-1.643151
C	1.191963	6.915303	7.583343
H	0.607380	6.118092	7.824858
H	0.887943	7.301207	6.688600
H	1.103459	7.633352	8.302617
C	8.971335	12.022722	3.107312
H	9.534805	12.817077	2.805463

H	9.583756	11.230652	3.295295
H	8.469222	12.271458	3.956989
C	-0.451139	8.293684	3.196470
H	-1.423535	7.999153	3.271841
H	-0.307244	8.752703	2.298689
H	-0.237912	8.952323	3.945511
C	1.861336	15.333981	6.242287
H	1.606379	16.318129	6.170956
H	1.539528	14.961996	7.133761
H	1.421887	14.817103	5.481759
C	3.280076	8.556741	-0.505237
H	2.975369	8.439215	-1.477326
H	4.146666	8.034292	-0.364103
C	4.776051	10.440735	-0.831408
H	4.862022	11.455600	-0.761926
H	4.748070	10.195836	-1.828190
C	9.203408	8.837551	1.277888
H	9.862853	8.067914	1.374839
H	9.711179	9.717210	1.223345
H	8.662381	8.711350	0.421754
C	2.902609	4.929038	4.003331
H	3.341644	4.042201	3.763562
H	1.907242	4.779352	4.167672
H	3.329950	5.309209	4.844442
C	-3.163610	9.516072	8.480583
H	-3.793741	8.715955	8.418769
H	-3.718705	10.372329	8.454869
H	-2.652985	9.475633	9.359461
C	7.680382	7.536093	2.740192
H	8.416515	6.827447	2.738510
H	6.996344	7.307695	2.022531
H	7.226344	7.540804	3.650925
C	-2.951566	9.237522	6.036844
H	-3.619183	8.481034	6.171602
H	-2.288135	8.983496	5.307821
H	-3.449942	10.080650	5.755934

Optimized structure of complex **3** assuming $5f^3$ configuration (U^{III})

92	2.716356000	10.872551000	6.901555000
92	3.320706000	10.177106000	2.680021000
45	5.387546000	9.339970000	4.837057000
45	2.577922000	13.164159000	4.594707000
45	3.387827000	7.914457000	4.997533000
45	0.613055000	11.681566000	4.769858000

15	1.496153000	13.122764000	2.439571000
15	2.178657000	7.063774000	3.164366000
15	3.616071000	14.072528000	6.518943000
15	-0.575225000	11.132580000	6.660856000
15	4.622918000	7.980285000	7.094647000
15	6.607114000	9.751658000	2.922427000
7	2.556993000	8.024415000	1.817977000
7	3.101539000	13.134405000	7.838975000
7	2.678556000	11.067242000	9.704028000
7	3.352615000	9.900122000	-0.118342000
7	2.087758000	11.918511000	1.394378000
7	4.116327000	9.215188000	8.149601000
7	0.504284000	10.601892000	7.886007000
7	5.521322000	10.082722000	1.653177000
6	5.522653000	14.188595000	6.659805000
1	5.695209000	14.669411000	7.631803000
6	1.471912000	10.326491000	10.105887000
1	1.272963000	10.448650000	11.186588000
1	1.665723000	9.264306000	9.928382000
6	6.117573000	12.785067000	6.719791000
1	7.210176000	12.831659000	6.809247000
1	5.878467000	12.200728000	5.820215000
1	5.738985000	12.228036000	7.582761000
6	7.308378000	8.783936000	7.399539000
1	8.339892000	8.564428000	7.703718000
1	6.924266000	9.597557000	8.020872000
1	7.338020000	9.138913000	6.355379000
6	-0.318062000	13.501246000	1.973611000
1	-0.276153000	13.906956000	0.954627000
6	3.738578000	6.310454000	7.520551000
1	4.072691000	5.646564000	6.712686000
6	-1.619487000	12.518914000	7.451418000
1	-1.947730000	12.108882000	8.414962000
6	3.155599000	15.936172000	6.629250000
1	3.549384000	16.308557000	5.672562000
6	3.904882000	10.445063000	10.226557000
1	3.855007000	10.342577000	11.326701000
1	4.732347000	11.126864000	10.001987000
6	7.911698000	11.149053000	2.925065000
1	8.477070000	11.003626000	1.995972000
6	0.226886000	10.714237000	9.303060000
1	-0.577551000	10.046275000	9.657382000
1	-0.090374000	11.728095000	9.601386000
6	2.265601000	7.715512000	0.437933000

1	2.365815000	6.644428000	0.193509000
1	1.235197000	7.987198000	0.140888000
6	6.438816000	7.536801000	7.500709000
1	6.425363000	7.200332000	8.545807000
6	3.823536000	14.630153000	2.285242000
1	4.369331000	15.579753000	2.217553000
1	4.251600000	13.927600000	1.563075000
1	4.039735000	14.214026000	3.292154000
6	3.466193000	13.388963000	9.216082000
1	3.266403000	14.421778000	9.542959000
1	4.540004000	13.218486000	9.425576000
6	4.214307000	9.092108000	9.587649000
1	5.217658000	8.795324000	9.942280000
1	3.525267000	8.335469000	10.001403000
6	2.327936000	14.825538000	2.054765000
1	1.939864000	15.480842000	2.845407000
6	-1.133609000	12.215532000	1.952497000
1	-2.168225000	12.416894000	1.647213000
1	-1.161122000	11.770626000	2.959924000
1	-0.704328000	11.473228000	1.274296000
6	2.613157000	12.482531000	10.105775000
1	2.893916000	12.599763000	11.167965000
1	1.575856000	12.810128000	10.004581000
6	7.711056000	8.227704000	2.549326000
1	8.220025000	8.067475000	3.509849000
6	0.262997000	7.066038000	3.369465000
1	0.078948000	6.747617000	4.404312000
6	2.508397000	5.225345000	2.771713000
1	1.845110000	4.982658000	1.932271000
6	3.797452000	16.738589000	7.762452000
1	3.565898000	17.804705000	7.639866000
1	4.886743000	16.646596000	7.792048000
1	3.407070000	16.436661000	8.738793000
6	-0.914116000	14.544542000	2.914936000
1	-1.966734000	14.730519000	2.666425000
1	-0.389207000	15.503612000	2.862656000
1	-0.863368000	14.187840000	3.951008000
6	3.951602000	5.003239000	2.340874000
1	4.097923000	3.965609000	2.014319000
1	4.635020000	5.195710000	3.173263000
1	4.235970000	5.666538000	1.520501000
6	7.229641000	12.508397000	2.859224000
1	7.974560000	13.313436000	2.821706000
1	6.599579000	12.673713000	3.737855000

1	6.590216000	12.584349000	1.976220000
6	2.033784000	15.465585000	0.698832000
1	2.544452000	16.435012000	0.624653000
1	0.966735000	15.654694000	0.550793000
1	2.385641000	14.847257000	-0.131488000
6	5.833666000	10.004701000	0.246586000
1	6.096990000	8.982094000	-0.076311000
1	6.688621000	10.636617000	-0.057228000
6	6.949346000	6.409573000	6.606809000
1	8.003283000	6.195208000	6.825465000
1	6.871009000	6.697611000	5.552082000
1	6.389715000	5.479088000	6.744138000
6	4.071562000	5.649104000	8.857938000
1	3.559882000	4.680278000	8.932935000
1	3.749647000	6.254955000	9.708954000
1	5.142097000	5.455097000	8.969344000
6	2.010835000	12.018714000	-0.047232000
1	2.768221000	12.704066000	-0.467290000
1	1.041298000	12.397470000	-0.415578000
6	6.157720000	15.050301000	5.571331000
1	7.249634000	15.064827000	5.679698000
1	5.813159000	16.088143000	5.610490000
1	5.936290000	14.662689000	4.572606000
6	-1.788130000	9.678395000	6.344273000
1	-1.073676000	8.908322000	6.028188000
6	-0.492797000	6.137803000	2.415356000
1	-1.575017000	6.266423000	2.546422000
1	-0.272218000	5.079923000	2.582169000
1	-0.265728000	6.368570000	1.368950000
6	-2.847833000	12.942045000	6.648152000
1	-3.257471000	13.871892000	7.063388000
1	-3.648039000	12.199048000	6.672667000
1	-2.590841000	13.136995000	5.601055000
6	-0.702437000	13.713724000	7.689889000
1	-1.191275000	14.450048000	8.341172000
1	-0.472001000	14.196119000	6.736635000
1	0.258110000	13.429047000	8.128652000
6	2.196024000	10.629003000	-0.661515000
1	1.304660000	10.036911000	-0.430437000
1	2.261609000	10.707184000	-1.762947000
6	2.239946000	6.551079000	7.352951000
1	1.672501000	5.616599000	7.447781000
1	1.981123000	6.969385000	6.354338000
1	1.859963000	7.268058000	8.087537000

6	8.866352000	11.030918000	4.111391000
1	9.633386000	11.814654000	4.069937000
1	9.384155000	10.066381000	4.136588000
1	8.330740000	11.146426000	5.059970000
6	-0.216560000	8.503416000	3.195265000
1	-1.298315000	8.567332000	3.348067000
1	0.001948000	8.863311000	2.184495000
1	0.270995000	9.192983000	3.906244000
6	1.641715000	16.110582000	6.614172000
1	1.376082000	17.168183000	6.488429000
1	1.198262000	15.762852000	7.551638000
1	1.190499000	15.535264000	5.798881000
6	3.271548000	8.465716000	-0.443151000
1	3.039913000	8.318505000	-1.514154000
1	4.256329000	8.031248000	-0.253222000
6	4.624743000	10.494414000	-0.560385000
1	4.541799000	11.576177000	-0.415369000
1	4.792532000	10.318433000	-1.639082000
6	8.771682000	8.399579000	1.460545000
1	9.318944000	7.457349000	1.327327000
1	9.510400000	9.167106000	1.708357000
1	8.329038000	8.656805000	0.493608000
6	2.145935000	4.349357000	3.970080000
1	2.299863000	3.289428000	3.731820000
1	1.104415000	4.468809000	4.284433000
1	2.783341000	4.592558000	4.827870000
6	-2.483896000	9.184131000	7.611116000
1	-3.095589000	8.300447000	7.386229000
1	-3.155588000	9.941143000	8.031767000
1	-1.761335000	8.899842000	8.378927000
6	6.808753000	7.028528000	2.286956000
1	7.392468000	6.099644000	2.254301000
1	6.283783000	7.128854000	1.331626000
1	6.048182000	6.942387000	3.068282000
6	-2.787454000	9.906812000	5.209106000
1	-3.184395000	8.946109000	4.857246000
1	-2.339017000	10.416419000	4.351658000
1	-3.643498000	10.502596000	5.535067000

Optimized structure of complex **3** assuming $5f^1$ configuration (U^V)

92	2.609217000	10.810824000	7.168953000
92	3.402837000	10.294761000	2.462830000
45	4.967822000	10.532850000	4.574868000
45	2.968517000	12.270838000	4.614937000

45	2.973119000	8.799361000	4.990984000
45	0.983887000	10.561270000	5.108418000
15	2.035829000	13.218231000	2.657485000
15	2.011932000	7.486657000	3.248328000
15	3.950865000	13.611729000	6.304014000
15	-0.562708000	10.612608000	6.825762000
15	3.873609000	7.873123000	6.971609000
15	6.577757000	10.343956000	2.930150000
7	2.484245000	8.353494000	1.784764000
7	3.417425000	12.826564000	7.787898000
7	2.697095000	11.123161000	9.837610000
7	3.433320000	10.017790000	-0.208848000
7	2.472935000	12.053331000	1.402347000
7	3.641864000	9.115240000	8.207706000
7	0.562380000	10.750402000	8.158834000
7	5.503225000	10.199851000	1.562274000
6	5.823153000	13.815839000	6.632274000
1	5.882658000	14.402313000	7.558147000
6	1.454331000	10.557150000	10.397137000
1	1.323353000	10.865254000	11.448172000
1	1.553401000	9.468904000	10.380933000
6	6.486624000	12.467470000	6.867888000
1	7.566754000	12.587320000	7.024827000
1	6.341533000	11.800576000	5.997337000
1	6.073275000	11.958910000	7.743733000
6	6.612667000	8.596867000	7.028019000
1	7.667203000	8.304295000	7.118272000
1	6.411872000	9.381452000	7.762567000
1	6.459643000	9.039287000	6.030169000
6	0.170216000	13.479274000	2.324140000
1	0.112242000	13.813440000	1.280376000
6	2.979531000	6.307993000	7.651772000
1	3.095510000	5.610017000	6.813212000
6	-1.773982000	12.066731000	7.063868000
1	-2.289500000	11.891430000	8.016295000
6	3.391073000	15.461713000	6.386902000
1	3.649537000	15.790549000	5.370479000
6	3.890989000	10.373298000	10.267777000
1	3.934020000	10.292755000	11.367372000
1	4.767339000	10.944952000	9.943911000
6	7.845089000	11.667264000	2.400848000
1	8.406535000	11.215532000	1.574126000
6	0.234283000	10.932478000	9.553985000
1	-0.590161000	10.287323000	9.889442000

1	-0.083037000	11.966724000	9.780250000
6	2.228521000	7.932457000	0.422401000
1	2.314340000	6.843092000	0.292429000
1	1.206812000	8.192835000	0.096512000
6	5.703553000	7.393935000	7.238623000
1	5.764433000	7.091146000	8.291900000
6	4.216243000	14.899163000	2.046362000
1	4.637477000	15.908117000	1.949655000
1	4.560106000	14.310211000	1.189801000
1	4.616534000	14.434930000	2.952293000
6	3.735828000	13.269490000	9.130269000
1	3.590000000	14.349274000	9.264591000
1	4.791156000	13.076572000	9.392267000
6	3.942644000	8.988444000	9.617398000
1	4.946138000	8.573128000	9.801194000
1	3.240963000	8.312345000	10.131173000
6	2.696862000	14.943477000	2.106631000
1	2.411430000	15.556342000	2.973185000
6	-0.590733000	12.172074000	2.457871000
1	-1.661502000	12.322766000	2.266751000
1	-0.476643000	11.760749000	3.474750000
1	-0.219466000	11.420039000	1.757811000
6	2.808719000	12.565721000	10.119922000
1	3.131892000	12.738241000	11.160348000
1	1.808047000	12.993321000	10.008660000
6	7.691310000	8.776924000	2.961190000
1	8.098028000	8.789644000	3.981033000
6	0.097636000	7.298441000	3.085118000
1	-0.198685000	6.974514000	4.090743000
6	2.527366000	5.673765000	2.884167000
1	2.021132000	5.388558000	1.954421000
6	4.069575000	16.407991000	7.380089000
1	3.748276000	17.439173000	7.181002000
1	5.160819000	16.394837000	7.315916000
1	3.791556000	16.187259000	8.415036000
6	-0.411480000	14.566055000	3.223803000
1	-1.475388000	14.716525000	3.000884000
1	0.088999000	15.531748000	3.102562000
1	-0.331183000	14.275718000	4.274939000
6	4.028365000	5.565491000	2.677684000
1	4.312422000	4.535931000	2.423523000
1	4.557199000	5.848638000	3.592042000
1	4.371839000	6.225784000	1.877318000
6	7.159923000	12.922453000	1.881897000

1	7.905135000	13.664901000	1.568737000
1	6.530234000	13.377549000	2.648411000
1	6.513405000	12.701644000	1.028695000
6	2.107059000	15.583424000	0.849235000
1	2.520189000	16.592782000	0.720557000
1	1.019130000	15.686034000	0.889808000
1	2.359402000	15.019275000	-0.053470000
6	5.885626000	10.025259000	0.180697000
1	6.130057000	8.974829000	-0.056965000
1	6.779444000	10.607314000	-0.094901000
6	6.098141000	6.206460000	6.365424000
1	7.139399000	5.919383000	6.559622000
1	6.013873000	6.457480000	5.305133000
1	5.474780000	5.326019000	6.550987000
6	3.538491000	5.627808000	8.902651000
1	2.984131000	4.699774000	9.096768000
1	3.437928000	6.250974000	9.795483000
1	4.592726000	5.354252000	8.801280000
6	2.274903000	12.213394000	-0.023464000
1	3.037384000	12.870639000	-0.473857000
1	1.303946000	12.670836000	-0.268049000
6	6.493620000	14.591694000	5.503884000
1	7.562916000	14.729466000	5.708523000
1	6.055996000	15.583624000	5.354269000
1	6.398974000	14.040974000	4.564636000
6	-1.637235000	9.078122000	7.280856000
1	-0.881686000	8.436824000	7.750393000
6	-0.417391000	6.270498000	2.073658000
1	-1.515219000	6.275739000	2.080257000
1	-0.102691000	5.247465000	2.293609000
1	-0.103953000	6.507481000	1.052323000
6	-2.801518000	12.097270000	5.934266000
1	-3.497459000	12.934733000	6.071067000
1	-3.396132000	11.179976000	5.885612000
1	-2.309225000	12.224293000	4.965116000
6	-0.987115000	13.366960000	7.151280000
1	-1.663161000	14.231053000	7.178566000
1	-0.323813000	13.469330000	6.287350000
1	-0.356162000	13.397499000	8.043248000
6	2.310092000	10.838831000	-0.699366000
1	1.386204000	10.306665000	-0.449611000
1	2.347808000	10.942161000	-1.797347000
6	1.496047000	6.632949000	7.793535000
1	0.913365000	5.728100000	8.009121000

1	1.112996000	7.089529000	6.873715000
1	1.327384000	7.346189000	8.608792000
6	8.812836000	11.962605000	3.545987000
1	9.573017000	12.687752000	3.229176000
1	9.337125000	11.065166000	3.891191000
1	8.283826000	12.385040000	4.404957000
6	-0.517946000	8.660502000	2.806176000
1	-1.613511000	8.609434000	2.826354000
1	-0.213328000	9.033403000	1.822806000
1	-0.201108000	9.401557000	3.559978000
6	1.875567000	15.513838000	6.525128000
1	1.507126000	16.541979000	6.416386000
1	1.557746000	15.141676000	7.504547000
1	1.400238000	14.891055000	5.762838000
6	3.252653000	8.584053000	-0.507621000
1	2.979211000	8.436392000	-1.565973000
1	4.218556000	8.098045000	-0.343224000
6	4.734725000	10.510595000	-0.703111000
1	4.707744000	11.602747000	-0.657960000
1	4.886586000	10.221664000	-1.756825000
6	8.852899000	8.722357000	1.968174000
1	9.372737000	7.760128000	2.063745000
1	9.597776000	9.505704000	2.133590000
1	8.507021000	8.797785000	0.931520000
6	2.056627000	4.758286000	4.011052000
1	2.353373000	3.720327000	3.813607000
1	0.971068000	4.771576000	4.148007000
1	2.510566000	5.062935000	4.958808000
6	-2.774382000	9.316572000	8.276434000
1	-3.224319000	8.356028000	8.559216000
1	-3.573559000	9.926263000	7.841571000
1	-2.449080000	9.805846000	9.197872000
6	6.788893000	7.561179000	2.812483000
1	7.323173000	6.639006000	3.072077000
1	6.437811000	7.464695000	1.780047000
1	5.904863000	7.650227000	3.450950000
6	-2.160012000	8.373575000	6.032362000
1	-2.655420000	7.431396000	6.300968000
1	-1.347384000	8.150064000	5.340788000
1	-2.891354000	8.988093000	5.495736000

Optimized structure of complex **2**

6	3.280545	10.914647	14.989778
1	2.831747	10.087988	15.631531
1	4.288986	10.916806	14.541788

6	3.160219	12.199719	15.756460
1	3.890158	12.920292	15.395855
1	3.378552	11.998193	16.802249
6	1.991716	9.407886	13.599739
1	2.771153	8.747330	13.984827
1	1.854121	9.181270	12.548066
6	0.685525	9.129412	14.336541
1	0.308776	8.155171	14.049518
1	0.850358	9.129868	15.412147
6	3.218792	11.300149	12.583305
1	4.055138	10.623795	12.397260
1	3.623309	12.276912	12.832643
6	2.376956	11.402659	11.324660
1	2.880067	12.029276	10.590014
1	2.245138	10.412682	10.891122
6	-2.101113	16.273775	15.399747
1	-2.612946	15.712587	14.629936
6	-2.520662	15.987615	16.691930
1	-3.289415	15.231255	16.752065
6	-2.545063	17.009603	17.819781
1	-3.416628	16.835697	18.442653
1	-2.627708	18.007535	17.402490
6	-1.278515	16.916134	18.682500
1	-1.424983	16.161164	19.448443
1	-1.108550	17.868529	19.183200
6	-0.046573	16.554736	17.867944
1	0.805564	16.284799	18.476476
6	0.303726	17.087482	16.595117
1	1.371450	17.130290	16.435462
6	-0.458850	18.180559	15.869129
1	0.235741	18.774092	15.284937
1	-0.929365	18.835156	16.596657
6	-1.532659	17.598481	14.924491
1	-2.345401	18.315883	14.823004
1	-1.096111	17.452513	13.942824
6	1.453503	13.011273	18.460457
1	2.440625	12.573861	18.580887
6	0.452372	11.865804	18.417785
1	0.459918	11.345049	19.373149
1	0.716682	11.169090	17.627830
1	-0.547086	12.246526	18.228976
6	1.195048	13.908614	19.696975
1	0.167810	14.262038	19.679957
1	1.867713	14.762348	19.687076

1	1.365116	13.326953	20.599766
6	2.991024	15.075050	17.010921
1	2.624288	15.959410	17.522141
6	4.216122	14.614039	17.821108
1	4.884470	14.039477	17.185698
1	3.912819	13.996739	18.661349
1	4.740030	15.489074	18.196343
6	3.416551	15.578200	15.612141
1	4.043339	16.460034	15.725420
1	2.540036	15.834429	15.024523
1	3.973975	14.804103	15.093950
6	-0.042523	13.902893	9.916306
1	-0.432247	14.600375	10.648277
6	-0.802119	14.180606	8.614554
1	-0.901178	15.254518	8.482603
1	-1.790365	13.734495	8.651576
1	-0.259161	13.765572	7.768669
6	1.456765	14.260508	9.760559
1	1.915108	13.626066	9.006038
1	1.964983	14.116156	10.708928
1	1.540754	15.301467	9.457749
6	-0.270933	10.944482	9.297447
1	-0.213869	9.965749	9.761299
6	0.919364	11.035599	8.309152
1	0.757755	10.333507	7.494789
1	1.846464	10.789448	8.817000
1	0.991240	12.041693	7.907929
6	-1.598060	10.982045	8.513865
1	-1.513097	11.669835	7.677811
1	-2.408566	11.309379	9.158681
1	-1.821679	9.987757	8.138039
6	-1.602296	8.565921	11.924091
1	-0.662930	8.704971	11.395016
6	-1.535577	7.159899	12.518064
1	-2.471152	6.918498	13.016008
1	-0.728340	7.082330	13.237514
1	-1.364843	6.443142	11.717944
6	-2.685398	8.627419	10.848879
1	-2.336919	8.120932	9.951753
1	-2.917139	9.659976	10.604638
1	-3.590251	8.140652	11.199715
6	-3.003199	9.612335	14.393570
1	-3.287775	10.562267	14.828366
6	-2.426409	8.776584	15.559164

1	-3.214442	8.597242	16.286590
1	-1.614323	9.320211	16.032271
1	-2.053077	7.824074	15.190950
6	-4.306539	8.978289	13.860047
1	-4.364261	9.065889	12.781411
1	-5.158154	9.490714	14.294852
1	-4.343891	7.925495	14.128550
17	-1.616852	13.062506	15.789765
17	0.450541	15.126826	13.414552
17	-3.033510	14.066290	11.097082
7	1.791976	12.795880	15.648173
7	-0.269580	10.175599	13.979963
7	1.092501	11.970740	11.687174
7	2.432844	10.801287	13.743509
15	1.476000	13.957360	16.845421
15	-1.695934	10.036569	13.104005
15	-0.265542	12.181367	10.709010
45	-0.482351	15.145867	16.365205
45	-2.127722	12.061166	12.067340
92	0.292127	12.429464	13.825572
6	-10.675162	15.298999	9.137165
1	-10.226970	16.125456	8.494770
1	-11.683149	15.297030	9.586233
6	-10.555827	14.013888	8.370894
1	-11.285136	13.293055	8.732321
1	-10.775705	14.215364	7.325257
6	-9.384189	16.806216	10.525459
1	-10.163916	17.467492	10.141783
1	-9.244850	17.032653	11.577109
6	-8.080419	17.083913	9.786124
1	-7.702576	18.057968	10.072495
1	-8.247409	17.084420	8.710873
6	-10.609003	14.914252	11.544328
1	-11.445009	15.590662	11.731645
1	-11.013856	13.937458	11.295778
6	-9.765583	14.811536	12.803523
1	-10.267399	14.184982	13.538760
1	-9.633575	15.801682	13.236618
6	-5.293188	9.939437	8.725543
1	-4.780304	10.500828	9.494505
6	-4.874734	10.224438	7.433440
1	-4.105744	10.980375	7.372145
6	-4.851871	9.201826	6.306132
1	-3.980664	9.375025	5.682570

1	-4.769399	8.204148	6.724064
6	-6.119033	9.295090	5.443777
1	-5.972887	10.049429	4.677176
1	-6.289467	8.342357	4.943908
6	-7.350072	9.657491	6.258766
1	-8.202445	9.927126	5.650531
6	-7.700178	9.126473	7.532504
1	-8.767796	9.084419	7.693033
6	-6.937253	8.033456	8.258708
1	-7.631715	7.440680	8.843879
1	-6.467738	7.378178	7.531156
6	-5.862162	8.615220	9.202103
1	-5.049792	7.897349	9.303314
1	-6.297854	8.761871	10.184034
6	-8.854554	13.200148	5.664484
1	-9.841818	13.637486	5.544930
6	-7.853455	14.345518	5.705142
1	-7.862195	14.866036	4.749627
1	-8.116656	15.042510	6.495298
1	-6.853722	13.964590	5.892665
6	-8.598414	12.301861	4.427756
1	-7.571065	11.948374	4.443046
1	-9.271118	11.448161	4.439700
1	-8.769998	12.882482	3.524590
6	-10.388409	11.138694	7.116394
1	-10.022410	10.254205	6.604830
6	-11.614136	11.599976	6.307445
1	-12.281625	12.174786	6.943550
1	-11.311174	12.217181	5.467027
1	-12.138828	10.725187	5.932608
6	-10.813080	10.635647	8.515433
1	-11.440301	9.753989	8.402726
1	-9.936242	10.379129	9.102257
1	-11.369795	11.410028	9.033975
6	-7.339639	12.306366	14.207100
1	-6.949692	11.610400	13.474505
6	-6.575547	12.030665	15.506127
1	-6.473043	10.956954	15.636491
1	-5.588600	12.479666	15.466636
1	-7.117465	12.443584	16.353670
6	-8.837652	11.945273	14.364979
1	-9.296461	12.577750	15.120815
1	-9.347989	12.089007	13.417779
1	-8.917778	10.903846	14.667042

6	-7.119500	15.266442	14.828581
1	-7.178755	16.245436	14.365543
6	-8.307619	15.174415	15.819813
1	-8.144832	15.876187	16.634180
1	-9.235937	15.420259	15.314118
1	-8.378044	14.168149	16.220836
6	-5.790220	15.228216	15.607242
1	-5.872193	14.539339	16.442645
1	-4.981337	14.901901	14.959017
1	-5.565831	16.222200	15.983218
6	-5.791434	17.646536	12.200194
1	-6.730008	17.506132	12.730337
6	-5.860651	19.051073	11.603906
1	-4.925776	19.293110	11.104977
1	-6.668444	19.126233	10.884846
1	-6.032005	19.768572	12.403260
6	-4.707411	17.591214	13.276022
1	-5.057230	18.099088	14.171988
1	-4.472125	16.560764	13.522857
1	-3.804206	18.080060	12.923813
6	-4.394510	16.604601	9.728249
1	-4.109364	15.654866	9.292791
6	-4.974343	17.440185	8.563746
1	-4.188007	17.621385	7.834955
1	-5.786426	16.895598	8.091537
1	-5.348602	18.391847	8.933198
6	-3.091066	17.241622	10.258873
1	-3.030982	17.153976	11.337387
1	-2.239096	16.731218	9.822273
1	-3.056091	18.294563	9.990536
17	-5.778118	13.150915	8.331890
17	-7.838316	11.087328	10.711182
17	-4.357495	12.147052	13.026230
7	-9.186768	13.418817	8.480090
7	-7.126100	16.035069	10.142870
7	-8.481011	14.242828	12.441774
7	-9.825386	15.412552	10.382623
15	-8.872699	12.256137	7.280240
15	-5.697924	16.176242	11.018516
15	-7.123180	14.031383	13.416418
45	-6.913072	11.067042	7.760660
45	-5.263018	14.152377	12.055387
92	-7.684820	13.784369	10.298087

5. References

1. Feng G, et al. (2019) Transition metal bridged bimetallic clusters with multiple uranium-metal bonds. *Nat Chem* 11:248-253.

2. Sheldrick GM (2000) SADABS, *Program for Empirical Absorption Correction of Area Detector Data*, University of Göttingen, Germany,.

3. Siemens (2000) *SHELXTL, Version 6.10,* Software Reference Manual, Siemens Analytical X-ray Systems, Inc., Madison, Wisconsin, USA,

4. Gaussian09, Revision A.02 (2009) Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery JA, Jr., Peralta JE, Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Rega N, Millam JM, Klene M, Knox JE, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski VG, Voth GA, Salvador P, Dannenberg JJ, Dapprich S, Daniels AD, Farkas O, Foresman JB, Ortiz JV, Cioslowski J, Fox DJ, Gaussian, Inc., Wallingford CT.

5. Becke AD (1993) Density-functional thermochemistry. III. The role of exact Exchange. *J Chem Phys* 98:5648–5652.

6. Perdew JP, Wang Y (1992) Accurate and simple analytic representation of the electron-gas correlation energy. *Phys Rev B* 45:13244–13249.

7. Cao X, Dolg M (2004) Segmented contraction scheme for small-core actinide pseudopotential basis set. *J Mol Struct: Theochem* 673:203–209.

8. Cao X, Dolg M, Stoll H (2003) Valence basis sets for relativistic energyconsistent small-core actinide pseudopotentials. *J Chem Phys* 118:487–496.

9. Kuechle W, Dolg M, Stoll H, Preuss H (1994) Energy-adjusted pseudopotentials for the actinides. Parameter sets and test calculations for thorium and thorium monoxide. *J Chem Phys* 100:7535–7542.

10. Leininger T, Nicklass A, Kuechle W, Stoll H, Dolg M, Bergner A (1996) The accuracy of the pseudopotential approximation: Non-frozen-core effects for spectroscopic constants of alkali fluorides XF (X = K, Rb, Cs). *Chem Phys Lett* 255:274–280.

11. Dolg M, Wedig U, Stoll H, Preuss H (1987) Energy-adjusted ab initio pseudopotentials for the first row transition elements. *J Chem Phys* 86:866–872.

12. Hehre WJ, Ditchfield R, Pople JA (1972) Self-consistent molecular orbital methods. XII. Further extensions of Gaussian-type basis sets for use in molecular orbital studies of organic molecules *J Chem Phys* 56:2257–2261.

13. Hariharan PC, Pople JA (1973) The influence of polarization functions on molecular orbital hydrogenation energies. *Theor Chim Acta* 28:213–222.

14. Schlegel HB (1982) Optimization of equilibrium geometries and transition structures. *J Comput Chem* 3:214–218.

15. Reed AE, Curtiss LA, Weinhold F (1988) Intermolecular interactions from a natural bond orbital, donor-acceptor viewpoint. *Chem Rev* 88:899–926.
16. Zhurko GA *Home Page: a set of graphical tools for facilitating working with quantum chemistry computations (*http://www.chemcraftprog.com).