# *NJC*

# **Evidence of the unprecedented conversion of intermolecular proton- to water-bridging two phosphoryl ruthenium complexes**

Rémy Sylvain,<sup>a</sup> LaureVendier,<sup>a</sup> Christian Bijani,<sup>a</sup> Antonio Santoro,<sup>b</sup> Fausto Punteriero,<sup>b</sup> Sebastiano Campagna,<sup>\*,b</sup> Pierre Sutra<sup>a</sup> and Alain Igau<sup>\*,a</sup>

# **Supporting information**

## SUMMARY

Experimental section : general information	3
Synthesis of complex [{ $[Ru](Ph_2P=O)$ } <sub>2</sub> H][PF <sub>6</sub> ] <sub>3</sub> <b>2</b> ([Ru]=Ru(tpy)(bpy))	5
Synthesis of complex $[{[Ru](Ph_2P=O)}_2(H_2O)][PF_6]_2$ 3 $([Ru]=Ru(tpy)(bpy))$	5
Figure S1. Molecular structure of complex 2	6
Table 1. Crystal data and structure refinement for complex 2	6
Table 2. Atomic coordinates and equivalent isotropic displacement parameters for	
complex <b>2</b>	7
Table 3. Bond lengths [A] and angles [deg] for complex 2.	9
Table 4. Anisotropic displacement parameters (A^2 x 10^3) for complex 2	15
Figure S2 : ${}^{31}P{}^{1}H$ NMR spectra of complex <b>2</b> in CD <sub>2</sub> Cl <sub>2</sub> at 233K	17
Figure S3 : <sup>1</sup> H NMR spectra of complex <b>2</b> in $CD_2Cl_2$ at 298K	17
Figure S4 : <sup>1</sup> H NMR spectra of complex <b>2</b> in $CD_2Cl_2$ at 233K.	18
Figure S5. Molecular structure of complex <b>3</b>	19
Figure S6. Packing of the molecular structure of complex <b>3</b> viewed along the C axis	19
Table 5. Crystal data and structure refinement for complex 3	20
Table 6. Atomic coordinates and equivalent isotropic displacement parameters for	
complex <b>3</b>	21
Table 7. Bond lengths [A] and angles [deg] for complex 3	22
Table 8. Anisotropic displacement parameters (A^2 x 10^3) for complex 3	26
Figure S7 : <sup>31</sup> P NMR spectra of complex <b>3</b> in CD <sub>3</sub> CN at 298K	28
Figure S8 : <sup>1</sup> H NMR spectra of complex <b>3</b> in $CD_2Cl_2$ at 298K	28
Figure S9 : <sup>1</sup> H NMR spectra of complex <b>3</b> in $CD_2Cl_2$ at 183K	29
Figure S10 : ${}^{1}H{}^{31}P{}$ et ${}^{1}H$ NMR spectra of complex <b>3</b> in CD <sub>2</sub> Cl <sub>2</sub>	
at 183K (17.0 ; 15.0ppm)	29
Figure S11. Luminescence spectra of <b>1</b> in acetonitrile at 298 K	
and in butyronitrile at 77 K	30
Table 9. Selected photophysical data of phosphoryl complexes 1, 2 and 3.	

## **Experimental Section**

### General Information.

All reactions were conducted under an inert atmosphere of dry argon using standard Schlenkline techniques. Solvents were dried, distilled, and degassed following conventional methods prior to use. Elemental analyses were carried out with a PerkinElmer 2400 Series II CHNS/O Elemental Analyzer. NMR spectra were recorded on a Bruker DPX 300, AV 300, AV 400 and on a Bruker AV 500 spectrometer. All the <sup>1</sup>H and <sup>13</sup>C signals were assigned on the basis of chemical shifts, spin-spin coupling constants, splitting patterns, and signal intensities and by using 2D experiments as <sup>1</sup>H-<sup>1</sup>H COSY45 and <sup>1</sup>H-<sup>13</sup>C HMQC experiments. Infrared spectra were recorded by using universal ATR sampling technology on a Perkin-Elmer spectrum 100 FT-IR. Mass spectra were recorded on a TSQ7000 instrument from ThermoElectron.

Data of compound 2 were collected at low temperature (180 K) on a Gemini Agilent diffractometer using a graphite-monochromated Cu-K $\alpha$  Enhance radiation ( $\lambda = 1.54184$  Å) and equipped with an Oxford Instrument Cooler Device. Indeed, it was really difficult to synthesise high diffracting crystals. In order to enhance the weak diffraction signal, we chose to record data under copper radiation.

Data of compound **3** were collected at low temperature (100 K) on a Bruker Kappa Apex II diffractometer using a graphite-monochromated Mo-K $\alpha$  radiation ( $\lambda = 0.71073$ Å) and equipped with an Oxford Cryosystems Cryostream Cooler Device.

The final unit cell parameters have been obtained by means of a least-squares refinement. The structures have been solved by Direct Methods using SIR92,<sup>1</sup> and refined by means of least-squares procedures on a F<sup>2</sup> with the aid of the program SHELXL97<sup>2</sup> include in the softwares package WinGX version 1.63.<sup>3</sup> The Atomic Scattering Factors were taken from International tables for X-Ray Crystallography.<sup>4</sup> All hydrogens atoms were geometrically placed and refined by using a riding model.

All non-hydrogens atoms were anisotropically refined, and in the last cycles of refinement a weighting scheme was used, where weights are calculated from the following formula: w=1/[ $\sigma^2(Fo^2)$ +(aP)<sup>2</sup>+bP] where P=(Fo<sup>2</sup>+2Fc<sup>2</sup>)/3.

Drawing of molecule are performed with the program ORTEP32<sup>5</sup> with 30% probability displacement ellipsoids for non-hydrogen atoms.

The electrochemical measurements were obtained using an Autolab PGSTAT 100 potentiostat using tetrabutylammonium hexafluorophosphate as the supporting electrolyte in freshly distilled acetonitrile and a platinum working electrode.

Absorption spectra were recorded with a Jasco V-560 spectrophotometer. For steady-state luminescence measurements, a Jobin Yvon-Spex Fluoromax P spectrofluorimeter was used, equipped with a Hamamatsu R3896 photomultiplier. The spectra were corrected for photomultiplier response using a program purchased with the fluorimeter. For the luminescence lifetimes, an Edinburgh OB 900 time-correlated single-photon-counting spectrometer was used. As excitation sources, a Hamamatsu PLP 2 laser diode (59 ps pulse width at 408 nm) and/or the nitrogen discharge (pulse width 2 ns at 337 nm) were employed.

Electrospray mass spectrometry analyses were performed on a Perkin Elmer Sciex API-365 spectrometer in positive mode. Melting points were determined in capillaries using an Electrothermal melting point apparatus.

The <sup>1</sup>H and <sup>13</sup>C are numbered as shown below.



 $\{[Ru(tpy)(bpy)(Ph_2PO)]_2H\}[PF_6]_3$  (2) : To a solution of  $[Ru(tpy)(bpy)(Ph_2PO)][PF_6]$  1 (0.100 g, 0.012 mmol) in 5 mL acetonitrile was added HCl (1 eq.) in Et<sub>2</sub>O and the mixture was stirred for 30 mn at room temperature. Addition of KPF<sub>6</sub> (1 eq) was followed and the cloudy mixture was filtered to remove the KCl salts. A large volume of ether (50 mL) was then added to the filtrate which was slowly reduced by two-thirds to give the product 2 as a red crystalline powder in 80% (81 mg) isolated yield, m. p. 168°C (dec).

NMR <sup>31</sup>P (121.5 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 213K) :  $\delta$  (ppm) = 112.2 (s), -144.2 (PF<sub>6</sub>, <sup>1</sup>J<sub>PF</sub>=704.6 Hz).

NMR <sup>1</sup>H (500MHz, CD<sub>2</sub>Cl<sub>2</sub>, 298K) :  $\delta$  (ppm) = 9.75 (d, 2H<sub>a</sub>, <sup>3</sup>J=5Hz), 8.48 (d, 2H<sub>d</sub>, <sup>3</sup>J=8Hz), 8.31 (d, 2H<sub>g</sub>, <sup>3</sup>J=8Hz), 8.20 (t, 2H<sub>c</sub>, <sup>3</sup>J=8Hz), 8.08-7.67 (m, 4H<sub>3</sub>, 4H<sub>3</sub>, 2H<sub>4</sub>', 4H<sub>4</sub>, 2H<sub>h</sub>, 2H<sub>b</sub>), 7.55 (d, 4H<sub>6</sub>, <sup>3</sup>J=5Hz), 7.21-7.16 (m, 4H<sub>5</sub>, 4H<sub>para</sub>, Ph, 2H<sub>i</sub>), 6.94 (m, 8H<sub>meta</sub>, Ph + 2Hj), 6.65 (dd, 8H<sub>ortho</sub>, Ph, <sup>3</sup>J=7.7Hz, <sup>3</sup>J=8Hz). NMR <sup>1</sup>H (500MHz, CD<sub>2</sub>Cl<sub>2</sub>, 213K) :  $\delta$  (ppm) = 10.06 (broad, H<sup>+</sup>), 9.75 (2H<sub>a</sub>), all the other signals are identicals to those observed at 298K.

NMR <sup>13</sup>C{<sup>1</sup>H} (75 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 213K) :  $\delta$  (ppm) = 156.1 (C<sub>a</sub>), 153.4 (C<sub>6</sub>), 148.2 (C<sub>j</sub>), 138.9 (C<sub>h</sub>), 138.0 (C<sub>c</sub>), 136.2 (C<sub>4</sub>'), 133.1 (C<sub>ipso</sub>, Ph), 130.4 (C<sub>para</sub>, Ph), 128.9 (C<sub>ortho</sub>, Ph), 128.6 (C<sub>meta</sub>, Ph), 128.4 (C<sub>4</sub>), 128.2 (C<sub>5</sub>), 127.8 (C<sub>b</sub>), 127.5 (C<sub>i</sub>), 124.3 (C<sub>3</sub>), 124.3 (C<sub>d</sub>), 123.6 (C<sub>g</sub>), 123.4 (C<sub>3'</sub>), the ipso carbon atoms in the tpy (C<sub>2</sub> and C<sub>2'</sub>) and bpy (C<sub>e</sub> and C<sub>f</sub>) ligands have not been observed.

Mass (ES<sup>+</sup>) :  $m/z = 692.1 [(2M-H^+-3PF_6)].$ 

 $\{[Ru(tpy)(bpy)(Ph_2PO)]_2H_2O\}[PF_6]_2$  (3) : In an acetonitrile solution (2 mL) of 2 (100 mg, 1.2 10-4 mol) was added water in excess followed by KPF<sub>6</sub> (0.221 mg, 1.2 10-3 mol). The reaction mixture was then stirred for 30 min. Complex 3 was isolated after filtration, washing with 3\*10 mL of water then 3\*10 mL of ether. The volatiles were evaporated and the product was isolated as a red solid in 91% (93 mg) yield, m. p. 142°C (dec).

RMN <sup>31</sup>P (121.5 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 298K) :  $\delta$  (ppm) = 95.3 (s), -144.4 (PF<sub>6</sub>, <sup>1</sup>J<sub>PF</sub>=704.6 Hz).

RMN <sup>1</sup>H (300MHz, CD<sub>2</sub>Cl<sub>2</sub>, 298K) :  $\delta$  (ppm) = 10.05 (d, 2H<sub>a</sub>, <sup>3</sup>*J*=5Hz), 8.47 (d, 2H<sub>d</sub>, <sup>3</sup>*J*=10Hz), 8.30 (d, 2H<sub>g</sub>, <sup>3</sup>*J*=10Hz), 8.21 (t, 2H<sub>c</sub>, <sup>3</sup>*J*=5Hz), 8.10-8.01 (m, 4H<sub>3+</sub>4H<sub>3'</sub>), 7.91 (t, 2H<sub>4'</sub>, <sup>3</sup>*J*=5Hz), 7.86 (t, 2H<sub>h</sub>, <sup>3</sup>*J*=5Hz), 7.60 (d, 4H<sub>6</sub>, <sup>3</sup>*J*=5Hz), 7.53 (t, 2H<sub>b</sub>, <sup>3</sup>*J*=5Hz), 7.28 (t, 4H<sub>5</sub>, <sup>3</sup>*J*=10Hz), 7.20 (t, 4H<sub>4</sub>, <sup>3</sup>*J*=5Hz), 7.16 (d, 2H<sub>j</sub>, <sup>3</sup>*J*=5Hz), 7.01-6.95 (m, 18H, H<sub>i</sub>+<sub>meta, ortho,</sub> Ph), 6.69 (t, 4H<sub>para</sub>, Ph, <sup>3</sup>*J*=10Hz).

NMR <sup>1</sup>H (500MHz, CD<sub>2</sub>Cl<sub>2</sub>, 183K) :  $\delta$  (ppm) = 16.17 (t broad, H<sub>2</sub>O).

RMN <sup>13</sup>C {<sup>1</sup>H}{<sup>31</sup>P} (75 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 298K) :  $\delta$  (ppm) = 156.1 (C<sub>a</sub>), 153.0 (C<sub>6</sub>), 148,0 (C<sub>j</sub>), 138.4 (C<sub>h</sub>), 137.8 (C<sub>c</sub>), 137.7 (C<sub>4</sub>'), 135.4 (C<sub>ipso</sub>, Ph), 129.8 (C<sub>4</sub>), 128.8 (C<sub>para</sub>, Ph), 128.7 (C<sub>ortho</sub>, Ph), 128.3 (C<sub>meta</sub>, Ph), 127.9 (C<sub>b</sub>), 127.2 (C<sub>i</sub>), 127.1 (C<sub>i</sub>), 123.9 (C<sub>3</sub>), 123.7 (C<sub>d</sub>), 123.2 (C<sub>g</sub>), 123.0 (C<sub>3</sub>'), the ipso carbon atoms in the tpy (C<sub>2</sub> and C<sub>2</sub>') and bpy (C<sub>e</sub> and C<sub>f</sub>) ligands have not been observed.

Mass (ES+) : m/z = 692 ([2M-H<sub>2</sub>O-2PF<sub>6</sub>)].

Elemental analysis Calcd. for: C<sub>74</sub>H<sub>60</sub>F<sub>12</sub>N<sub>10</sub>O<sub>3</sub>P<sub>4</sub>Ru<sub>2</sub> (1692,17): C, 52.55; H, 3.58; N, 8.28. Found: C, 52.74; H, 3.79; N, 8.07.



Figure S1. Molecular structure of complex 2.

#### Table 1. Crystal data and structure refinement for complex 2.

```
Identification code
                                    remy240112
                                    C74 H59 N10 O2 P2 Ru2, 3(F6 P)
Empirical formula
Formula weight
                                    1819.30
Temperature
                                    180(2) K
Wavelength
                                    1.54180 A
Crystal system, space group
                                    Monoclinic, C 1 2/c 1
Unit cell dimensions
                                                alpha = 90 deg.
beta = 100.457(3) deg.
gamma = 90 deg.
                            a
b
C
                                17.2568(6) A
                              = 29.2556(13) A
= 15.1819(5) A
Volume
                                    7537.4(5) A^3
Z, Calculated density
                                    4, 1.603 Mg/m^3
Absorption coefficient
                                    5.115 mm^-1
F(000)
                                    3656
                                    0.15 x 0.06 x 0.03 mm
Crystal size
Theta range for data collection
                                    3.88 to 60.82 deg.
Limiting indices
                                    -19<=h<=19, -32<=k<=29, -15<=1<=17
Reflections collected / unique
                                    16962 / 5658 [R(int) = 0.0402]
Completeness to theta = 60.82
                                    98.4 %
Absorption correction
                                    Semi-empirical from equivalents
Max. and min. transmission
                                    0.8657 and 0.5714
Refinement method
                                    Full-matrix least-squares on F^2
                                    5658 / 0 / 513
Data / restraints / parameters
Goodness-of-fit on F^2
                                    1.051
                                    R1 = 0.0681, wR2 = 0.1900
Final R indices [I>2sigma(I)]
R indices (all data)
                                    R1 = 0.0866, wR2 = 0.2074
Largest diff. peak and hole
                                    1.559 and -0.986 e.A^-3
```

### Table 2. Atomic coordinates and equivalent isotropic displacement parameters for complex 2.

	x	У	Z	U(eq)
C(11)	898(4)	779(3)	100(4)	31(2)
C(12)	516(4)	449(3)	-477(5)	33(2)
C(13)	823(4)	15(3)	-451(4)	30(2)
C(14)	1519(4)	-81(3)	131(1) 126(4)	30(2) 31(2)
C(14)	1888(1)	263(3)	675(4)	30(2)
C(15)	2657(4)	203(3)	1290(5)	30(2)
C(10)	2037(4)	203(3)	1421 (J)	32(2)
C(17)	3100(4)	-192(3)	1431(J) 2057(5)	42(2)
C(10)	3790(4)	-100(3)	2037(3) 2502(5)	44(2)
C(19)	4029(4) 2505(4)	211(3)	2302(5) 2220(E)	4/(2)
C(20)	3585(4)	603(3)	2329(5)	39(2)
C(21)	3/56(5)	1061(3)	2/18(6)	4/(2)
C(22)	4448(5)	11/0(4)	3314(6)	61(3)
C(23)	45/2(6)	1611(5)	3610(8)	83(4)
C(24)	4015(7)	1937(4)	3320(7)	/3(3)
C(25)	3325(6)	1815(3)	2737(6)	58(2)
C(1)	3309(5)	1225(3)	148(6)	47(2)
C(2)	3522(5)	1386(4)	-630(6)	56(2)
C(3)	3082(6)	1719(3)	-1112(6)	61(3)
C(4)	2439(6)	1901(3)	-800(6)	52(2)
C(5)	2255(5)	1738(3)	-3(5)	41(2)
C(6)	1619(5)	1917(3)	411(5)	40(2)
C(7)	1114(6)	2264(3)	39(6)	53(2)
C(8)	546(6)	2424(3)	481(7)	59(2)
C(9)	487(6)	2243(3)	1300(6)	57(2)
C(10)	987(6)	1896(3)	1636(6)	52(2)
C(26)	1662(5)	1115(3)	3737(5)	39(2)
C(27)	1014(5)	1227(3)	4136(5)	41(2)
C(28)	1139(6)	1376(3)	5024(6)	53(2)
C(29)	1892(6)	1406(3)	5515(6)	56(2)
C(30)	2530(6)	1306(3)	5128(6)	51(2)
C(31)	2414(5)	1161(3)	4242(5)	44(2)
C(32)	1648(4)	271(3)	2833(4)	29(2)
C(33)	2330(4)	100(3)	3375(5)	34(2)
C(34)	2454(4)	-365(3)	3486(5)	38(2)
C(35)	1899(5)	-672(3)	3074(5)	41(2)
C(36)	1212(4)	-513(3)	2537(5)	36(2)
C(37)	1096(4)	-48(3)	2411(4)	31(2)
N(3)	1574(3)	690(2)	673(4)	29(1)
N(4)	2897(3)	591(2)	1734(4)	34(1)
N(5)	3190(4)	1385(2)	2441(4)	46(2)
N(1)	2689(4)	1401(2)	454(4)	42(2)
N(2)	1545(4)	1718(2)	1207(4)	39(2)
F(13)	4543(3)	337(2)	575(3)	61(1)
F(14)	5180(3)	-345(2)	827(3)	63(2)
F(15)	4193(3)	-262(2)	-370(3)	63(2)
P(1)	1495(1)	876(1)	2595(1)	31(1)
P(2)	0	1835(1)	7500	97(2)
P(3)	4686(3)	-1586(2)	2169(4)	69(2)
P(4)	5000	0	0	51(1)

 $\ensuremath{\text{U}}\left(\ensuremath{\text{eq}}\right)$  is defined as one third of the trace of the orthogonalized Uij tensor.

#### Electronic Supplementary Material (ESI) for New Journal of Chemistry This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

Ru(1)	2226(1)	1137(1)	1557(1)	33(1)
F(1)	145(5)	1457(3)	8239(4)	110(3)
F(2A)	423(8)	2275(4)	7974(8)	95(2)
F(3A)	969(8)	1690(4)	7460(8)	95(2)
F(3B)	-233(11)	2080(6)	8498(11)	95(2)
F(2B)	759(11)	1995(6)	7772(11)	95(2)
F(7)	5111(10)	-1146(5)	2226(17)	166(8)
F(9)	5065(15)	-1647(5)	1612(18)	470(20)
F(8)	3945(12)	-1302(5)	2172(14)	298(12)
F(10)	4376(10)	-1979(6)	2406(19)	166(8)
0(1)	601(3)	926(2)	2200(3)	34(1)

$\alpha(11)$ $N(2)$	1 240(0)
C(11) - N(3)	1.340(9)
C(11)-C(12)	1.388(10)
C(11) = H(11)	0 9500
C(II) - H(II)	0.9500
C(12)-C(13)	1.373(10)
C(12) = U(12)	0 9500
C(12) - H(12)	0.9500
C(13)-C(14)	1.381(10)
C(12) $T(12)$	0 0500
C(13) - H(13)	0.9500
C(14)-C(15)	1.385(10)
C(14) = H(14)	0 9500
$C(14)^{-11}(14)$	0.9500
C(15)-N(3)	1.359(9)
C(15) = C(16)	1 /89(10)
C(15) = C(10)	1.409(10)
C(16)-N(4)	1.347(9)
C(16) = C(17)	1 381(11)
	1.301(11)
C(17)-C(18)	1.382(11)
C(17) - H(17)	0 9500
	0.9900
C(18)-C(19)	1.368(12)
C(18) - H(18)	0 9500
0(10) m(10)	1.001(10)
C(19) - C(20)	1.381(12)
С(19)-Н(19)	0.9500
C(20) N(4)	1 255/01
$\cup (\angle \cup) = \mathbb{N}(4)$	1.300(9)
C(20)-C(21)	1.472(12)
C(21) = N(5)	1 270 (11)
C(ZT) - IN(Z)	1.3/U(11)
C(21)-C(22)	1.398(12)
C(22) = C(23)	1 368(15)
$\cup (\angle \angle ) = \cup (\angle \cup )$	T.300(T3)
С(22)-Н(22)	0.9500
C(23) - C(24)	1 369(17)
C(23) = C(24)	1.309(17)
С(23)-Н(23)	0.9500
C(24) - C(25)	1 396(14)
C(24) $C(25)$	1.330(14)
C(24)-H(24)	0.9500
C(25) - N(5)	1 344(11)
C(25) N(5)	1.911(11)
С(25)-Н(25)	0.9500
C(1) - N(1)	1.344(11)
C(1) = C(2)	1 202 (12)
C(1) = C(2)	1.382(12)
C(1)-H(1)	0.9500
C(2) $C(2)$	1 262(14)
C(2) = C(3)	1.303(14)
C(2)-H(2)	0.9500
C(3) - C(4)	1 389(17)
С(З)-Н(З)	0.9500
C(4) - C(5)	1 391 (11)
$\sim$ $(1)$ $\sim$ $(0)$	
C(4) - H(4)	0.9500
C(5)-N(1)	1.352(11)
C(E) = C(E)	1 457 (11)
C(5) = C(6)	1.45/(11)
C(6)-N(2)	1.368(10)
C(G) = C(T)	1 200 (12)
C(6) = C(7)	1.390(12)
C(7) - C(8)	1.367(13)
C(7) = U(7)	0 9500
$C(7) = \Pi(7)$	0.9300
C(8)-C(9)	1.373(13)
C(8) = H(8)	0 9500
C(9)-C(10)	1.371(13)
C(9) - H(9)	0.9500
$\sim \langle \mathcal{I} \rangle$ $\rightarrow \langle \mathcal{I} \rangle$	
C(10) - N(2)	1.361(11)
С(10)-Н(10)	0.9500
C(26) = C(21)	1 200 (10)
C(20) = C(31)	1.309(12)
C(26)-C(27)	1.405(11)
C(26) - P(1)	1 8/2 (0)
C(20) = P(1)	⊥.04∠(ŏ)
C(27)-C(28)	1.397(11)
C(27) = U(27)	0 0500
$\bigcirc$ $( \angle I ) = \Pi ( \angle I )$	0.3000

Table 3. Bond lengths [A] and angles [deg] for complex 2.

C(12)-C(11)-H(11)	119.0
C(13) – C(12) – C(11) C(13) – C(12) – H(12)	120.4
С(11)-С(12)-Н(12)	120.4
C(12)-C(13)-C(14)	119.5(7)
C(12) - C(13) - H(13)	120.2
C(14) - C(13) - R(13) C(13) - C(14) - C(15)	119.1(7)
C(13) -C(14) -H(14)	120.5
C(15)-C(14)-H(14)	120.5
N(3) - C(15) - C(14)	121.7(6)
N(3) = C(15) = C(16) C(14) = C(15) = C(16)	114.8(6) 123.4(7)
N(4) - C(16) - C(17)	121.1(7)
N(4)-C(16)-C(15)	111.8(6)
C(17)-C(16)-C(15)	127.1(7)
C(16) - C(17) - C(18) C(16) - C(17) - H(17)	118.6(8)
C(18) - C(17) - H(17) C(18) - C(17) - H(17)	120.7
C(19) -C(18) -C(17)	119.7(8)
С(19)-С(18)-Н(18)	120.1
C(17) - C(18) - H(18)	120.1
C(18) - C(19) - C(20) C(18) - C(19) - H(19)	120.3(0)
С(20) –С(19) –Н(19)	119.8
N(4)-C(20)-C(19)	119.5(8)
N(4) - C(20) - C(21)	112.4(7)
C(19) = C(20) = C(21) N(5) = C(21) = C(22)	128.1(7) 121.3(9)
N(5) - C(21) - C(20)	115.1(7)
C(22)-C(21)-C(20)	123.6(9)
C(23) -C(22) -C(21)	119.4(10)
C(23) = C(22) = H(22) C(21) = C(22) = H(22)	120.3
C(22) - C(22) - C(24)	119.5(10)
С(22) –С(23) –Н(23)	120.2
С(24)-С(23)-Н(23)	120.2
C(23) = C(24) = C(25) C(23) = C(24) = H(24)	119.6(10)
C(25) - C(24) - H(24)	120.2
N(5)-C(25)-C(24)	121.8(10)
N(5)-C(25)-H(25)	119.1
C(24) - C(25) - H(25)	119.1 121.1(9)
N(1) = C(1) = C(2) N(1) = C(1) = H(1)	119.4
C(2) - C(1) - H(1)	119.4
C(3)-C(2)-C(1)	119.6(9)
C(3) - C(2) - H(2)	120.2
C(2) = C(2) = H(2) C(2) = C(3) = C(4)	120.2
С(2) –С(3) –Н(3)	120.2
С(4)-С(3)-Н(3)	120.2
C(3) - C(4) - C(5)	119.2(9)
C(3) = C(4) = H(4) C(5) = C(4) = H(4)	120.4 120.4
N(1) - C(5) - C(4)	120.3(8)
N(1)-C(5)-C(6)	115.6(7)
C(4) - C(5) - C(6)	124.1(8)
N(2) = C(6) = C(7) N(2) = C(6) = C(5)	121.2(7) 115-2(7)
C(7) - C(6) - C(5)	123.6(7)

C(8) = C(7) = C(6)	120 2(8)
	120.2(0)
C(8) - C(7) - H(7)	119.9
C(6) - C(7) - H(7)	119.9
C(7) - C(8) - C(9)	119 4 (9)
	100 0
C(7) - C(8) - H(8)	120.3
С(9)-С(8)-Н(8)	120.3
C(10) - C(9) - C(8)	118 6(9)
C(10) C(0) U(0)	120.7
C(10) = C(9) = H(9)	120.7
С(8)-С(9)-Н(9)	120.7
N(2) - C(10) - C(9)	123.9(8)
N(2) = C(10) = H(10)	118 1
N(2) = C(10) = H(10)	110.1
C(9) - C(10) - H(10)	118.1
C(31)-C(26)-C(27)	118.4(7)
C(31) - C(26) - P(1)	121 9(6)
C(21) = C(20) = (1)	110 C(C)
C(27) = C(26) = P(1)	119.0(0)
C(28)-C(27)-C(26)	119.6(8)
С(28)-С(27)-Н(27)	120.2
C(26) - C(27) - H(27)	120 2
C(20) = C(27) = H(27)	120.2
C(29) - C(28) - C(27)	120.5(8)
С(29)-С(28)-Н(28)	119.8
C(27) - C(28) - H(28)	119 8
	100 5 (0)
C(30) = C(29) = C(28)	120.5(8)
С(30)-С(29)-Н(29)	119.8
С(28)-С(29)-Н(29)	119.8
C(29) - C(30) - C(31)	119 6(9)
C(20) = C(20) = U(20)	120.2
C(29) = C(30) = H(30)	120.2
С(31)-С(30)-Н(30)	120.2
C(26)-C(31)-C(30)	121.4(8)
С(26)-С(31)-Н(31)	119.3
C(30) - C(31) - H(31)	119 3
C(22) C(22) C(27)	117 4(7)
C(33) = C(32) = C(37)	11/.4(/)
C(33) - C(32) - P(1)	122.7(6)
C(37)-C(32)-P(1)	119.7(5)
C(34) - C(33) - C(32)	121.1(7)
C(24) - C(22) - H(22)	110 /
C(34) = C(33) = H(33)	119.4
С (32) – С (33) – Н (33)	119.4
C(35)-C(34)-C(33)	120.5(7)
C(35) - C(34) - H(34)	119.8
C(22) - C(24) - H(24)	110.0
$C(33) = C(34) = \Pi(34)$	119.0
C(34) - C(35) - C(36)	119.6(/)
С(34)-С(35)-Н(35)	120.2
С (36) – С (35) – Н (35)	120.2
C(37) - C(36) - C(35)	119 9(7)
	100 1
C(37) - C(36) - H(36)	120.1
С(35)-С(36)-Н(36)	120.1
C(36)-C(37)-C(32)	121.4(7)
C(36) = C(37) = H(37)	110 3
	110 0
C(32) = C(37) = H(37)	119.3
C(11)-N(3)-C(15)	118.5(6)
C(11)-N(3)-Ru(1)	127.1(5)
$C(15) = N(3) = B_{11}(1)$	1143(4)
C(15) N(5) Ru(1)	124.5(4)
C(16) - N(4) - C(20)	120.6(7)
C(16)-N(4)-Ru(1)	119.9(5)
C(20)-N(4)-Ru(1)	119.5(5)
C(25) - N(5) - C(21)	118.3(8)
$C(25) = N(5) = D_{11}(1)$	128 0 (7)
C(2J) = N(J) = Ru(1)	$\pm 20.0(7)$
C(21) - N(5) - Ru(1)	LL3.7(5)
C(1)-N(1)-C(5)	120.2(7)
C(1)-N(1)-Ru(1)	124.8(6)
$C(5) - N(1) - B_{11}(1)$	114 6(5)
C(10) = N(2) = C(6)	116 C (J)
$\cup (\bot \cup) = \mathbb{N} (Z) = \cup (b)$	ттр.р(/)

Q (10) N (0) D (1)	
C(10) = N(2) = Ru(1)	127.3(5)
C(6)-N(2)-Ru(1)	115.8(5)
O(1) - P(1) - C(32)	105 3 (3)
O(1) P(1) O(02)	107 (2)
O(1) = P(1) = C(26)	107.6(3)
C(32)-P(1)-C(26)	101.0(3)
O(1)-P(1)-Ru(1)	109.33(19)
C(22) = D(1) = D(1)	110 2(2)
C(32) = P(1) = Ru(1)	112.3(2)
C(26)-P(1)-Ru(1)	120.2(2)
F(2B)-P(2)-F(2B)#1	140.4(15)
F(2B) - P(2) - F(1) # 1	118 3(8)
$\Gamma(2D) = \Gamma(2) + \Gamma(1) + 1$	110.0(0)
F(ZB) # I - P(Z) - F(I) # I	90.3(8)
F(2B)-P(2)-F(1)	90.3(8)
F(2B)#1-P(2)-F(1)	118.3(8)
F(1) # 1 - P(2) - F(1)	89 9(6)
$\Gamma(T) \parallel T(T) = \Gamma(T)$	
F(ZB) - P(Z) - F(ZA) # I	101.1(10)
F(2B)#1-P(2)-F(2A)#1	42.0(8)
F(1)#1-P(2)-F(2A)#1	104.3(5)
F(1) - P(2) - F(2A) # 1	$154\ 2(6)$
E(2D) D(2) E(2D)	42 0 (9)
F(2B) = P(2) = F(2A)	42.0(0)
F(2B)#1-P(2)-F(2A)	101.1(10)
F(1)#1-P(2)-F(2A)	154.2(6)
F(1) - P(2) - F(2A)	$104 \ 3(5)$
	71 5(9)
F(2A) # I - F(2) - F(2A)	150.0(9)
F(2B) - P(2) - F(3A) #1	159.8(9)
F(2B)#1-P(2)-F(3A)#1	39.3(8)
F(1)#1-P(2)-F(3A)#1	79.8(5)
F(1) - P(2) - F(3A) # 1	80 4 (5)
$\Gamma(1) = (2) + (31) + 1$	
F(2A) # I - P(2) - F(3A) # I	81.2(6)
F(2A)-P(2)-F(3A)#1	123.2(7)
F(2B)-P(2)-F(3A)	39.3(8)
F(2B)#1-P(2)-F(3A)	159.8(9)
$\nabla (1) \# 1 - \nabla (2) - \nabla (3\pi)$	80 4 (5)
F(1) # 1 - F(2) - F(3A)	00.4(5)
F'(1) - P(2) - F'(3A)	/9.8(5)
F(2A)#1-P(2)-F(3A)	123.2(7)
F(2A)-P(2)-F(3A)	81.2(6)
F(3A) #1 - P(2) - F(3A)	151 8 (9)
E(2D) = C(2) = C(2D) = 1	
F(2B) = P(2) = F(3B) # I	76.7(9)
F(2B)#1-P(2)-F(3B)#1	87.6(10)
F(1)#1-P(2)-F(3B)#1	73.0(6)
F(1) - P(2) - F(3B) #1	149.5(7)
$\Sigma(2\pi) + 1 - D(2) - \Sigma(2D) + 1$	56 2 (7)
F(2A) # I = P(2) = F(3B) # I	56.5(7)
F(2A)-P(2)-F(3B)#1	84.4(7)
F(3A)#1-P(2)-F(3B)#1	119.6(7)
F(3A)-P(2)-F(3B)#1	72.6(7)
F(2B) = P(2) = F(3B)	87 6(10)
$\Gamma(2D) I(2) \Gamma(3D)$	
$F_{1}(ZB) # T - F_{1}(Z) - F_{2}(ZB)$	/6./(9)
F(1)#1-P(2)-F(3B)	149.5(7)
F(1)-P(2)-F(3B)	73.0(6)
F(2A)#1-P(2)-F(3B)	84,4(7)
$r(2\pi) = r(2) = r(3\pi)$	563(7)
F(2A) = F(2) = F(3B)	50.5(7)
F(3A) # I - P(2) - F(3B)	/2.6(/)
F(3A)-P(2)-F(3B)	119.6(7)
F(3B)#1-P(2)-F(3B)	132.6(12)
F(9) - P(3) - P(3) # 2	93 4 (17)
= (0) = D(3) = E(10)	111 E/1/V
F(2) = F(2) = F(10)	111.0(14)
P(3)#2-P(3)-F(10)	96.1(12)
F(9)-P(3)-F(7)	80.6(9)
P(3)#2-P(3)-F(7)	68.3(9)
F(10) - P(3) - F(7)	161.4(17)
= (-2) = (-2) = (-2)	101 //101
F(J) = F(J) = F(0)	101.4(18)
₽(3)#Z−₽(3)−F(8)	124.3(11)

F(10)-P(3)-F(8)	95.2(8)
F(7)-P(3)-F(8)	86.1(10)
F(9)-P(3)-F(7)#2	116.5(9)
P(3)#2-P(3)-F(7)#2	60.1(10)
F(10)-P(3)-F(7)#2	126.7(15)
F(7)-P(3)-F(7)#2	37.0(14)
F(8)-P(3)-F(7)#2	69.7(11)
F(9)-P(3)-F(9)#2	131.0(13)
P(3)#2-P(3)-F(9)#2	39.8(7)
F(10)-P(3)-F(9)#2	71.3(13)
F(7)-P(3)-F(9)#2	90.1(13)
F(8)-P(3)-F(9)#2	95.3(9)
F(7)#2-P(3)-F(9)#2	60.4(11)
F(9)-P(3)-F(10)#2	67.7(15)
P(3)#2-P(3)-F(10)#2	42.0(6)
F(10)-P(3)-F(10)#2	76.1(9)
F(7)-P(3)-F(10)#2	96.8(8)
F(8)-P(3)-F(10)#2	160.8(10)
F(7) #2 - P(3) - F(10) #2	101.5(10)
F(9) #2 - P(3) - F(10) #2	65.8(8)
F(14) #3-P(4) - F(14)	180.0(4)
F(14) #3 - P(4) - F(15) #3	90.3(3)
F(14) - P(4) - F(15) #3	89.7(3)
F(14) # 3 - P(4) - F(15)	89.7(3)
F(14) - P(4) - F(15)	90.3(3)
F'(15) # 3 - P(4) - F'(15)	180.0(6)
F'(14) # 3 - P(4) - F'(13)	89.7(3)
F(14) - F(4) - F(13)	90.3(3)
F(15) = F(4) = F(13) F(15) = F(4) = F(12)	89.8(3)
r(13) = r(4) = r(13)	90.2(3)
F(14) - F(4) - F(13) #3	89 7 (3)
F(15) #3 - P(4) - F(13) #3	90.2(3)
F(15) - P(4) - F(13) #3	89.8(3)
F(13) - P(4) - F(13) #3	180.0(4)
N(4) - Ru(1) - N(3)	79.1(2)
N(4)-Ru(1)-N(5)	79.2(3)
N(3) -Ru(1) -N(5)	157.8(3)
N(4)-Ru(1)-N(2)	172.8(2)
N(3)-Ru(1)-N(2)	97.8(2)
N(5)-Ru(1)-N(2)	103.3(3)
N(4)-Ru(1)-N(1)	96.1(3)
N(3)-Ru(1)-N(1)	87.5(2)
N(5)-Ru(1)-N(1)	90.6(2)
N(2)-Ru(1)-N(1)	77.2(3)
N(4)-Ru(1)-P(1)	91.05(17)
N(3)-Ru(1)-P(1)	86.16(15)
N(5)-Ru(1)-P(1)	98.45(17)
N(2) - Ru(1) - P(1)	95.24(17)
N(1) - Ru(1) - P(1)	169.34(19)
E'(/)#2-E'(/)-P(3)	//.4(/)
F(7) #2 - F(7) - F(3) #2	65.6(1/)
r (こ) = r ( / ) = F (こ) 冊乙 R (フ) #つ - R (フ) - R (ロ)	31.7(0)
r (/ ) # ∠ - r (/ ) - r (ツ) P ( 3 ) - 〒 ( 7 ) - 〒 ( 9 )	$\perp \perp \circ \cdot \angle (\circ)$ $12 \circ (7)$
ェ 、J /	42.0(7)
F(7)#2-F(7)-F(8)#2	92 (3)
P(3) - F(7) - F(8) # 2	101.9(8)
P(3) #2-F(7) -F(8) #2	53.7(7)
F(9) - F(7) - F(8) #2	90.5(13)
P(3) - F(9) - F(7)	57.4(6)
· · · ·	· · ·

Symmetry transformations used to generate equivalent atoms: #1 -x, y, -z+3/2 #2 -x+1, y, -z+1/2 #3 -x+1, -y, -z

#### Table 4. Anisotropic displacement parameters $(A^2 \times 10^3)$ for complex 2.

The anisotropic displacement factor exponent takes the form: -2 pi^2 [ h^2 a\*^2 U11 + ... + 2 h k a\* b\* U12 ]

	U11	U22	U33	U23	U13	U12
C(11)	38(4)	36(4)	23(4)	1 (3)	13(3)	0(3)
C(12)	31(4)	50(5)	21(3)	2(3)	12(3)	-1(3)
C(13)	28(4)	43(4)	22(3)	-3(3)	9(3)	-11(3)
C(14)	36(4)	36(4)	26(4)	-2(3)	20(3)	-6(3)
C(15)	30(4)	40(4)	22(3)	-2(3)	15(3)	-5(3)
C(16)	30(4)	47(4)	24(3)	0(3)	15(3)	-3(3)
C(17)	36(4)	62 (5)	32(4)	0(4)	19(3)	7(4)
C(18)	32(4)	70(6)	35(4)	1(4)	19(3)	11(4)
C(19)	27(4)	83(7)	35(4)	0(4)	19(3)	-3(4)
C(20)	29(4)	63 (5)	30(4)	-5(4)	17(3)	-9(4)
C(21)	37(4)	68(6)	41(5)	-2(4)	21(4)	-12(4)
C(22)	34(5)	98(8)	49(5)	-20(5)	7 (4)	-19(5)
C(23)	52(6)	110(10)	81(8)	-21(7)	-1(6)	-34(7)
C(24)	73(7)	76(7)	68(7)	-21(6)	6(6)	-40(6)
C(25)	70(6)	61(6)	45(5)	-2(5)	12(5)	-20(5)
C(1)	45(5)	61(6)	39(5)	-10(4)	21(4)	-21(4)
C(2)	54(5)	72(7)	50(5)	-9(5)	29(5)	-26(5)
C(3)	84(7)	65(6)	41(5)	0(5)	31(5)	-34(6)
C(4)	78(6)	46(5)	38(5)	2(4)	25(4)	-25(5)
C(5)	51(5)	39(4)	35(4)	-3(4)	14(4)	-20(4)
C(6)	58(5)	36(4)	28(4)	-5(3)	13(4)	-15(4)
C(7)	75(6)	43(5)	43(5)	5(4)	18(5)	-10(5)
C(8)	73(6)	45(5)	60(6)	7 (5)	16(5)	0(5)
C(9)	71(6)	43(5)	62(6)	-1(4)	27(5)	6(5)
C(10)	75(6)	39(5)	46(5)	0(4)	26(5)	-2(4)
C(26)	51(5)	36(4)	34(4)	-1(3)	19(4)	-8(3)
C(27)	53(5)	38(4)	37(4)	-4(3)	21(4)	-3(4)
C(28)	75(6)	50(5)	41(5)	-19(4)	28(5)	-7(5)
C(29)	87(7)	47(5)	36(5)	-18(4)	20(5)	-23(5)
C(30)	69(6)	51(5)	36(5)	-8(4)	16(4)	-19(4)
C(31)	53(5)	48(5)	35(4)	-6(4)	17(4)	-15(4)
C(32)	30(4)	45(4)	18(3)	1(3)	15(3)	-1(3)
C(33)	28(4)	53(5)	24(4)	-6(3)	15(3)	-1(3)
C(34)	31(4)	58(5)	29(4)	4(4)	14(3)	9(4)
C(35)	49(5)	41(4)	37(4)	4(4)	22(4)	5(4)
C(36)	39(4)	42(5)	30(4)	-1(3)	15(3)	-1(3)
C(37)	31(4)	45(4)	21(3)	-1(3)	13(3)	-6(3)
N(3)	32(3)	40(3)	20(3)	1(3)	17(2)	-2(3)
N(4)	25(3)	54(4)	24(3)	-2(3)	10(2)	-9(3)
N(5)	51(4)	53(4)	38(4)	-10(3)	20(3)	-27(4)

N(1)	44(4)	53(4)	32(3)	-4(3)	16(3)	-22(3)
N(2)	54(4)	37(4)	29(3)	-4(3)	14(3)	-12(3)
F(13)	43(3)	104(4)	41(3)	-2(3)	19(2)	11(3)
F(14)	52(3)	104(4)	35(3)	14(3)	15(2)	8(3)
F(15)	36(2)	112(4)	42(3)	3(3)	13(2)	3(3)
P(1)	33(1)	39(1)	24(1)	-3(1)	14(1)	-5(1)
P(2)	123(4)	44(2)	97(3)	0	-54(3)	0
P(3)	84(4)	63(3)	76(4)	24(3)	60(3)	27(3)
P(4)	31(2)	96(3)	30(2)	7(2)	13(1)	9(2)
Ru(1)	37(1)	41(1)	25(1)	-3(1)	15(1)	-10(1)
F(1)	150(7)	129(6)	53(4)	17(4)	26(4)	2(5)
F(2A)	117(6)	81(5)	79(5)	-19(4)	-6(4)	12(4)
F(3A)	117(6)	81(5)	79(5)	-19(4)	-6(4)	12(4)
F(3B)	117(6)	81(5)	79(5)	-19(4)	-6(4)	12(4)
F(2B)	117(6)	81(5)	79(5)	-19(4)	-6(4)	12(4)
F(7)	110(8)	105(8)	330(20)	131(11)	175(12)	74(7)
F(9)	730(40)	188(13)	700(40)	-255(19)	700(40)	-242(19)
F(8)	400(20)	202(13)	390(20)	146(15)	320(20)	157(15)
F(10)	110(8)	105(8)	330(20)	131(11)	175(12)	74(7)
0(1)	33(3)	41(3)	30(3)	0(2)	17(2)	2(2)



Figure S2 :  ${}^{31}P{}^{1}H$  NMR spectra of complex 2 in CD<sub>2</sub>Cl<sub>2</sub> at 233K.



Figure S3 : <sup>1</sup>H NMR spectra of complex **2** in  $CD_2Cl_2$  at 298K.



Figure S4 : <sup>1</sup>H NMR spectra of complex 2 in  $CD_2Cl_2$  at 233K.



Figure S5. Molecular structure of complex **3**.



Figure S6. Packing of the molecular structure of complex **3** viewed along the C axis.

### Table 5. Crystal data and structure refinement for complex 3.

Identification code	rsi070212
Empirical formula	2(C37 H29 N5 O P Ru), 2(F6 P), H2 O
Formula weight	1691.34
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group Unit cell dimensions	Tetragonal, I 41 c d a = 28.4278(6) A alpha = 90 deg. b = 28.4278(6) A beta = 90 deg. c = 17.0604(4) A gamma = 90 deg.
Volume	13787.2(5) A^3
Z, Calculated density	8, 1.630 Mg/m^3
Absorption coefficient	0.622 mm^-1
F(000)	6832
Crystal size	0.15 x 0.03 x 0.02 mm
Theta range for data collection	2.00 to 21.70 deg.
Limiting indices	-29<=h<=29, -29<=k<=28, -17<=1<=17
Reflections collected / unique	98325 / 4063 [R(int) = 0.0583]
Completeness to theta = $21.70$	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.989 and 0.812
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4063 / 1 / 477
Goodness-of-fit on F^2	1.056
<pre>Final R indices [I&gt;2sigma(I)]</pre>	R1 = 0.0163, $wR2 = 0.0349$
R indices (all data)	R1 = 0.0195, $wR2 = 0.0360$
Absolute structure parameter	-0.032(16)
Largest diff. peak and hole	0.150 and -0.147 e.A^-3

Table 6. Atomic coordinates and equivalent isotropic displacement parameters for complex 3. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

$\begin{array}{cccccc} C(1) & 10267(1) & 7546(1) & 11067(2) & 22(1) \\ C(3) & 9521(1) & 7914(1) & 1132(2) & 30(1) \\ C(4) & 9325(1) & 7445(1) & 10398(2) & 30(1) \\ C(4) & 9325(1) & 7445(1) & 11321(2) & 25(1) \\ C(5) & 9616(1) & 7090(1) & 11378(2) & 17(1) \\ C(6) & 9439(1) & 6615(1) & 11551(2) & 16(1) \\ C(7) & 8966(1) & 6503(1) & 11550(2) & 20(1) \\ C(8) & 8823(1) & 6049(1) & 11724(2) & 21(1) \\ C(9) & 9161(1) & 5715(1) & 11890(2) & 19(1) \\ C(10) & 9631(1) & 5843(1) & 11870(2) & 17(1) \\ C(11) & 10421(1) & 6048(1) & 9997(2) & 18(1) \\ C(12) & 10557(1) & 5966(1) & 9236(2) & 20(1) \\ C(13) & 10966(1) & 6187(1) & 8965(2) & 21(1) \\ C(14) & 11217(1) & 6479(1) & 9465(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10223(2) & 16(1) \\ C(16) & 11289(1) & 6851(1) & 10737(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(19) & 11596(1) & 7444(1) & 11982(2) & 26(1) \\ C(20) & 11205(1) & 7159(1) & 12294(2) & 20(1) \\ C(21) & 10905(1) & 7130(1) & 12784(2) & 20(1) \\ C(22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7302(1) & 14106(2) & 34(1) \\ C(24) & 10320(1) & 7003(1) & 14033(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(23) & 10695(1) & 7362(1) & 13046(2) & 19(1) \\ C(25) & 10245(1) & 6772(1) & 13614(2) & 30(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 26(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 26(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 28(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 28(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 28(1) \\ C(33) & 11816(1) & 6081(1) & 11794(2) & 30(1) \\ C(33) & 11816(1) & 6081(1) & 11794(2) & 31(1) \\ C(33) & 11816(1) & 6081(1) & 11794(2) & 31(1) \\ C(33) & 11816(1) & 6081(1) & 11774(1) & 34(1) \\ C(33) & 11816(1) & 6081(1) & 11773(2) & 28(1) \\ C(33) & 11816(1) & 6081(1) & 11774(1) & 14(1) \\ N(4) & 11067(1) & 6886(1) & 11774(1) & 34(1) \\ C(33) & 11816(1) & 6081(1) & 11773(1) & 23(1) \\ F(4) & 1266(1) & 6622(1) & 17735(1) & 23(1) \\ F(4) & 1266(1) & 6622(1) & 17735(1) & 23(1) $		х	У	Z	U(eq)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(1)	10267(1)	7546(1)	11067(2)	22(1)
$\begin{array}{ccccc} C(2) & 9998(1) & 7945(1) & 10989(2) & 30(1) \\ C(4) & 9325(1) & 7485(1) & 11321(2) & 25(1) \\ C(5) & 9616(1) & 7090(1) & 11378(2) & 17(1) \\ C(6) & 9439(1) & 6615(1) & 11551(2) & 16(1) \\ C(7) & 8966(1) & 6503(1) & 11560(2) & 20(1) \\ C(8) & 8223(1) & 6049(1) & 11724(2) & 21(1) \\ C(9) & 9161(1) & 5715(1) & 11890(2) & 19(1) \\ C(10) & 9631(1) & 5843(1) & 11870(2) & 17(1) \\ C(11) & 10421(1) & 6048(1) & 9997(2) & 18(1) \\ C(12) & 10567(1) & 5966(1) & 9236(2) & 19(1) \\ C(13) & 10968(1) & 6187(1) & 8965(2) & 21(1) \\ C(14) & 11217(1) & 6479(1) & 9465(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10023(2) & 16(1) \\ C(16) & 11289(1) & 6851(1) & 10797(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(21) & 10905(1) & 7130(1) & 12784(2) & 20(1) \\ C(22) & 10905(1) & 7302(1) & 1406(2) & 34(1) \\ C(24) & 10320(1) & 7033(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13314(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 11204(1) & 6633(1) & 13519(2) & 26(1) \\ C(30) & 10688(1) & 5365(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5416(1) & 10737(2) & 42(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(33) & 10651(1) & 5436(1) & 110737(2) & 42(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(34) & 12250(1) & 6356(1) & 11444(2) & 31(1) \\ C(35) & 12335(1) & 5681(1) & 10922(2) & 40(1) \\ C(36) & 11978(1) & 5365(1) & 11248(1) & 17(1) \\ N(2) & 9779(1) & 6281(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5433(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5433(1) & 10737(2) & 42(1) \\ C(36) & 11978(1) & 5755(1) & 17605(1) & 28(1) \\ F(4) & 10684(1) & 7755(1) & 1775(1) & 28(1) \\ F(4) & 10684(1) & 7755(1) & 1775(1) & 28(1) \\ F(4) & 10684(1) & 7755(1) & 1775(1) & 25(1) \\ F(4) & 10684(1) & 5722(1) & 11660(1) & 277(1) \\ F(4) & 10684(1) & 5822(1) & 11999(1) & 16(1) \\ F(4) & 10684(1) & 5822(1) & 11999(1) & 16(1) \\ F(4) & 10684(1) & 582(1) & 17755(1) & 23(1) \\ F($	C(3)	9521(1)	7914(1)	11132(2)	30(1)
$\begin{array}{cccc} C(4) & 9325(1) & 7485(1) & 11321(2) & 25(1) \\ C(5) & 9616(1) & 7090(1) & 11378(2) & 17(1) \\ C(6) & 9439(1) & 6615(1) & 11551(2) & 16(1) \\ C(7) & 8966(1) & 6503(1) & 11560(2) & 20(1) \\ C(8) & 8823(1) & 6049(1) & 11724(2) & 21(1) \\ C(9) & 9161(1) & 5715(1) & 11890(2) & 19(1) \\ C(10) & 9631(1) & 5843(1) & 11870(2) & 17(1) \\ C(11) & 10421(1) & 6048(1) & 9997(2) & 18(1) \\ C(12) & 10567(1) & 5966(1) & 9236(2) & 19(1) \\ C(13) & 10968(1) & 6187(1) & 8965(2) & 21(1) \\ C(14) & 11217(1) & 6479(1) & 9465(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10223(2) & 16(1) \\ C(16) & 11289(1) & 6861(1) & 10797(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(19) & 11596(1) & 7159(1) & 12091(2) & 19(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(21) & 10905(1) & 7302(1) & 14409(2) & 34(1) \\ C(24) & 10320(1) & 7032(1) & 14409(2) & 34(1) \\ C(25) & 10245(1) & 7302(1) & 14409(2) & 34(1) \\ C(26) & 10925(1) & 5766(1) & 133619(2) & 26(1) \\ C(26) & 10925(1) & 5776(1) & 13341(2) & 23(1) \\ C(27) & 11204(1) & 6633(1) & 14687(2) & 43(1) \\ C(30) & 10688(1) & 5355(1) & 114249(2) & 41(1) \\ C(31) & 10668(1) & 5356(1) & 114249(2) & 41(1) \\ C(33) & 11816(1) & 6081(1) & 13719(2) & 23(1) \\ C(33) & 11816(1) & 6081(1) & 13719(2) & 21(1) \\ C(33) & 11816(1) & 6081(1) & 10737(2) & 42(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 21(1) \\ C(33) & 11816(1) & 6081(1) & 10737(2) & 42(1) \\ C(33) & 11816(1) & 6336(1) & 10737(2) & 42(1) \\ C(34) & 12250(1) & 6336(1) & 10737(2) & 42(1) \\ C(35) & 12335(1) & 5681(1) & 10737(2) & 42(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5369(1) & 10737(2) & 42(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5369(1) & 10737(2) & 42(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ F(4) & 12666(1) & 6224(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6224(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6224(1) & 17735(1) & 23(1) \\ F(4) & 12666(1) & 6221(1) & 11625(1) & 44(1) \\ F(4) & 12666(1) & 6221(1) & 11625(1) &$	C(2)	9998(1)	7945(1)	10989(2)	30(1)
$\begin{array}{ccccc} C(5) & 9616(1) & 7090(1) & 11378(2) & 17(1) \\ C(6) & 9439(1) & 6615(1) & 11551(2) & 16(1) \\ C(7) & 8966(1) & 6503(1) & 11560(2) & 20(1) \\ C(8) & 8823(1) & 6049(1) & 11724(2) & 21(1) \\ C(10) & 9631(1) & 5715(1) & 11890(2) & 19(1) \\ C(11) & 10421(1) & 6048(1) & 9997(2) & 18(1) \\ C(12) & 10567(1) & 5966(1) & 9236(2) & 19(1) \\ C(13) & 10968(1) & 6187(1) & 8965(2) & 21(1) \\ C(14) & 11217(1) & 6479(1) & 9465(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10223(2) & 16(1) \\ C(16) & 11289(1) & 6861(1) & 10797(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(19) & 11596(1) & 7444(1) & 11982(2) & 26(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(22) & 10958(1) & 7302(1) & 14106(2) & 34(1) \\ C(24) & 10320(1) & 7303(1) & 14039(2) & 31(1) \\ C(25) & 1025(1) & 7302(1) & 14106(2) & 34(1) \\ C(25) & 1025(1) & 5766(1) & 13064(2) & 19(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 10204(1) & 5633(1) & 14487(2) & 43(1) \\ C(27) & 10204(1) & 5635(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5345(1) & 14487(2) & 43(1) \\ C(33) & 11646(1) & 5345(1) & 11794(1) & 31(1) \\ C(33) & 11646(1) & 5345(1) & 11704(1) & 14(1) \\ C(31) & 10668(1) & 5345(1) & 11444(2) & 31(1) \\ C(33) & 11846(1) & 6035(1) & 11444(2) & 31(1) \\ C(34) & 12250(1) & 6035(1) & 11444(2) & 31(1) \\ C(35) & 12335(1) & 568(1) & 1777(2) & 28(1) \\ N(1) & 10084(1) & 7175(1) & 1268(1) & 171(1) \\ N(3) & 10651(1) & 6336(1) & 10488(1) & 14(1) \\ N(4) & 10651(1) & 6336(1) & 11704(1) & 4(1) \\ N(4) & 10651(1) & 6336(1) & 11704(1) & 4(1) \\ N(4) & 10651(1) & 6336(1) & 11704(1) & 4(1) \\ F(3) & 11903(1) & 6322(1) & 1775(1) & 23(1) \\ F(4) & 1266(1) & 6624(1) & 17735(1) & 23(1) \\ F(4) & 1266(1) & 6628(1) & 17735(1) & 23(1) \\ F(4) & 1266(1) & 6628(1) & 17735(1) & 23(1) \\ F(4) & 1266(1) & 6628(1) & 17735(1) & 23(1) \\ F(4) & 1266(1) & 6521(1) & 11625(1) & 44(1) \\ F(3) & 11903(1) & 6322(1) & 11625(1) & 44(1) \\ F(4) & 1266(1) & 638(1) & 17735(1) & 23(1) \\ F(4) & 1266($	C(4)	9325(1)	7485(1)	11321(2)	25(1)
$\begin{array}{cccc} C(6) & 9439(1) & 6615(1) & 11551(2) & 16(1) \\ C(7) & 8966(1) & 6503(1) & 11560(2) & 20(1) \\ C(8) & 8823(1) & 6049(1) & 11724(2) & 21(1) \\ C(10) & 9631(1) & 5715(1) & 11890(2) & 19(1) \\ C(11) & 10421(1) & 6048(1) & 9997(2) & 18(1) \\ C(12) & 10567(1) & 5966(1) & 9236(2) & 19(1) \\ C(13) & 10968(1) & 6187(1) & 8965(2) & 20(1) \\ C(14) & 11217(1) & 6479(1) & 9465(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10223(2) & 16(1) \\ C(16) & 11289(1) & 6851(1) & 1077(2) & 28(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(22) & 10905(1) & 7130(1) & 12784(2) & 20(1) \\ C(22) & 10905(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7302(1) & 14106(2) & 34(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13644(2) & 19(1) \\ C(29) & 10964(1) & 5655(1) & 14249(2) & 41(1) \\ C(29) & 10964(1) & 5655(1) & 14249(2) & 41(1) \\ C(30) & 10688(1) & 5365(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5365(1) & 114249(2) & 41(1) \\ C(33) & 11816(1) & 6081(1) & 1379(2) & 28(1) \\ C(33) & 11816(1) & 6081(1) & 1379(2) & 28(1) \\ C(33) & 11816(1) & 6081(1) & 1793(2) & 28(1) \\ N(1) & 10084(1) & 777(2) & 11614(2) & 18(1) \\ C(35) & 12335(1) & 5661(1) & 1077(2) & 42(1) \\ C(36) & 11978(1) & 5369(1) & 1077(2) & 42(1) \\ C(37) & 11534(1) & 5369(1) & 10737(2) & 42(1) \\ N(3) & 10651(1) & 6336(1) & 10488(1) & 14(1) \\ N(4) & 11067(1) & 688(1) & 1775(1) & 23(1) \\ F(4) & 1266(1) & 6736(1) & 1774(1) & 35(1) \\ F(4) & 1266(1) & 6736(1) & 1775(1) & 23(1) \\ F(4) & 1266(1) & 6736(1) & 1775(1) & 23(1) \\ F(4) & 1266(1) & 6744(1) & 15822(2) & 35(1) \\ F(4) & 1266(1) & 6744(2) & 11625(1) & 44(1) \\ F(4) & 1266(1) & 6724(1) & 1775(1) & 23(1) \\ F(4) & 1266(1) & 6724(1) & 1775(1) & 23(1) \\ F(4) & 1266(1) & 6724(1) & 1775(1) & 23(1) \\ $	C(5)	9616(1)	7090(1)	11378(2)	17(1)
$\begin{array}{cccccc} C(7) & 8966(1) & 6503(1) & 11560(2) & 20(1) \\ C(8) & 8823(1) & 6049(1) & 11724(2) & 21(1) \\ C(10) & 9631(1) & 5715(1) & 11890(2) & 19(1) \\ C(11) & 10421(1) & 6048(1) & 9997(2) & 18(1) \\ C(12) & 10567(1) & 5966(1) & 9236(2) & 19(1) \\ C(13) & 10968(1) & 6187(1) & 8965(2) & 21(1) \\ C(14) & 11217(1) & 6479(1) & 9465(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10223(2) & 16(1) \\ C(16) & 11289(1) & 6861(1) & 10797(2) & 18(1) \\ C(16) & 11289(1) & 6861(1) & 10797(2) & 29(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(19) & 11596(1) & 7444(1) & 11982(2) & 26(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(21) & 10905(1) & 7130(1) & 12784(2) & 20(1) \\ C(22) & 10905(1) & 7130(1) & 12784(2) & 20(1) \\ C(22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 11204(1) & 6063(1) & 13519(2) & 26(1) \\ C(29) & 10964(1) & 5633(1) & 14687(2) & 43(1) \\ C(33) & 11668(1) & 5355(1) & 14249(2) & 41(1) \\ C(33) & 11668(1) & 5365(1) & 11264(2) & 18(1) \\ C(33) & 11616(1) & 6081(1) & 11793(2) & 23(1) \\ C(33) & 11816(1) & 6081(1) & 10737(2) & 42(1) \\ C(33) & 11836(1) & 5365(1) & 110444(2) & 31(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(33) & 11836(1) & 5365(1) & 11249(2) & 40(1) \\ C(33) & 11836(1) & 5365(1) & 11249(2) & 40(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(35) & 12335(1) & 5681(1) & 10922(2) & 40(1) \\ C(37) & 11534(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5369(1) & 10737(2) & 42(1) \\ F(3) & 100631(1) & 6320(1) & 12716(1) & 18(1) \\ N(4) & 10651(1) & 638(1) & 1775(1) & 23(1) \\ F(4) & 1266(1) & 7145(1) & 1770(1) & 35(1) \\ F(4) & 1266(1) & 7145(1) & 1770(1) & 35(1) \\ F(5) & 11668(1) & 7145(1) & 1775(1) & 23(1) \\ F(4) & 1266(1) & 6388(1) & 17735(1) & 23(1) \\ F(4) & 1266(1) & 6380(1) & 14323(2) & 3$	C(6)	9439(1)	6615(1)	11551(2)	16(1)
$\begin{array}{cccc} C(8) & 8823(1) & 6049(1) & 11724(2) & 21(1) \\ C(9) & 9161(1) & 5715(1) & 11890(2) & 19(1) \\ C(10) & 9631(1) & 5843(1) & 11870(2) & 17(1) \\ C(11) & 10421(1) & 6048(1) & 9997(2) & 18(1) \\ C(12) & 10567(1) & 5966(1) & 9236(2) & 21(1) \\ C(13) & 10968(1) & 6187(1) & 8965(2) & 21(1) \\ C(14) & 11227(1) & 6479(1) & 9465(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10223(2) & 16(1) \\ C(16) & 11289(1) & 6861(1) & 10797(2) & 18(1) \\ C(16) & 11289(1) & 6861(1) & 10797(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7302(1) & 14106(2) & 34(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 11204(1) & 6063(1) & 13519(2) & 26(1) \\ C(29) & 10964(1) & 5663(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5416(1) & 13441(2) & 30(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(35) & 12335(1) & 568(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5413(1) & 11079(2) & 28(1) \\ N(1) & 10054(1) & 5376(1) & 11744(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 10488(1) & 17(1) \\ N(4) & 10651(1) & 6336(1) & 11746(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5475(1) & 17605(1) & 28(1) \\ N(4) & 10651(1) & 6336(1) & 10737(2) & 42(1) \\ F(4) & 12666(1) & 622(1) & 17745(1) & 18(1) \\ O(1) & 10594(1) & 5775(1) & 17605(1) & 28(1) \\ F(4) & 12666(1) & 6622(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6632(1) & 17745(1) & 35(1) \\ F(5) & 11668(1) & 7145(1) & 17735(1) & 23(1) \\ F(6) & 12134(1) & 6814(1) & 16806(1) & 47(1) \\ F(4) & 1266(1) & 6821(1) & 17735(1) & 23(1) \\ F(6) & 12134(1) & 6814(1) & 16806(1) & 27(1) \\ F(4) & 1226(1) & 6888(1) & 17735(1) & 23(1) \\ F(6) & 12134(1) & 6814(1) & 16686(1) & 27(1) \\ $	C(7)	8966(1)	6503(1)	11560(2)	20(1)
$\begin{array}{cccc} C(9) & 9161(1) & 5715(1) & 11890(2) & 19(1) \\ C(10) & 9631(1) & 5843(1) & 11870(2) & 17(1) \\ C(11) & 10421(1) & 6048(1) & 9997(2) & 18(1) \\ C(12) & 10567(1) & 5966(1) & 9236(2) & 29(1) \\ C(13) & 10968(1) & 6187(1) & 8965(2) & 20(1) \\ C(14) & 11217(1) & 6479(1) & 9455(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10223(2) & 16(1) \\ C(16) & 11289(1) & 6861(1) & 10797(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7449(1) & 11282(2) & 26(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(21) & 11596(1) & 7144(1) & 11982(2) & 26(1) \\ C(22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7302(1) & 14039(2) & 31(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 11204(1) & 6063(1) & 13519(2) & 23(1) \\ C(30) & 10688(1) & 5365(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5416(1) & 13441(2) & 30(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(35) & 12335(1) & 5681(1) & 10922(2) & 40(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5413(1) & 11079(2) & 23(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5413(1) & 11079(2) & 23(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5413(1) & 11794(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 10488(1) & 17(1) \\ N(4) & 10651(1) & 6336(1) & 1048(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 1048(1) & 14(1) \\ N(4) & 10651(1) & 6336(1) & 10737(2) & 42(1) \\ F(1) & 10530(1) & 6830(1) & 12716(1) & 18(1) \\ O(1) & 10594(1) & 5775(1) & 17605(1) & 28(1) \\ F(4) & 1266(1) & 6624(1) & 17745(1) & 35(1) \\ F(5) & 11668(1) & 7145(1) & 17735(1) & 23(1) \\ F(6) & 12134(1) & 6814(1) & 16626(1) & 47(1) \\ F(3) & 11903(1) & 6322(1) & 17860(1) & 42(1) \\ F(4) & 1266(1) & 6624(1) & 17735(1) & 23(1) \\ F(6) & 12134(1) & 6614(1) & 16625(1) & 44(1) \\ F(2) & 12126(1) & 6888(1) & 17735(1) & 23(1) \\ F(6) & 12124(1) & 6008(1) & 14323(2) & 35(1) \\ F(6) & 12124(1) & 6008(1) & 14323(2) & 35(1) $	C(8)	8823(1)	6049(1)	11724(2)	21(1)
$\begin{array}{ccccc} C(10) & 9631(1) & 5843(1) & 11870(2) & 17(1) \\ C(11) & 10421(1) & 6048(1) & 9997(2) & 18(1) \\ C(12) & 10567(1) & 5966(1) & 9236(2) & 19(1) \\ C(13) & 10968(1) & 6187(1) & 8965(2) & 20(1) \\ C(14) & 11217(1) & 6479(1) & 9465(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10233(2) & 16(1) \\ C(16) & 11289(1) & 6861(1) & 10797(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(19) & 11596(1) & 7444(1) & 11982(2) & 26(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(21) & 10995(1) & 7367(1) & 13479(2) & 28(1) \\ C(22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7302(1) & 14106(2) & 31(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(29) & 10964(1) & 5663(1) & 14687(2) & 43(1) \\ C(30) & 10668(1) & 5345(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5345(1) & 14249(2) & 41(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(34) & 12250(1) & 6636(1) & 10922(2) & 40(1) \\ C(35) & 12335(1) & 5681(1) & 10922(2) & 40(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 28(1) \\ N(1) & 10084(1) & 7125(1) & 11268(1) & 17(1) \\ N(2) & 9779(1) & 6281(1) & 10737(2) & 28(1) \\ N(1) & 10053(1) & 6336(1) & 10488(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 10488(1) & 14(1) \\ N(4) & 11067(1) & 6868(1) & 11499(1) & 16(1) \\ N(5) & 10530(1) & 6330(1) & 2776(1) & 118(1) \\ O(1) & 10594(1) & 7376(1) & 1776(1) & 28(1) \\ F(1) & 12430(1) & 7375(1) & 17605(1) & 28(1) \\ F(2) & 12292(1) & 6953(1) & 18606(1) & 27(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(5) & 11668(1) & 7145(1) & 17720(1) & 35(1) \\ F(6) & 12134(1) & 6814(1) & 16806(1) & 27(1) \\ F(4) & 12666(1) & 6624(1) & 17735(1) & 23(1) \\ F(6) & 12134(1) & 6814(1) & 16806(1) & 27(1) \\ F(4) & 12266(1) & 6888(1) & 17735(1) & 23(1) \\ F(6) & 12134(1) & 6814(1) & 16806(1) & 27(1) \\ F(1) & 1084(1) & 522(1) & 11625(1) & 14(1) \\ C(28) & 11224(1) & 6008(1) & 14323(2) & 35(1) \\ F(2) & 10000 & 5000 & 10634(2) & 25(1) \\ \end{array} \right)$	C(9)	9161(1)	5715(1)	11890(2)	19(1)
$\begin{array}{ccccc} C(11) & 10421(1) & 6048(1) & 9997(2) & 18(1) \\ C(12) & 10567(1) & 5966(1) & 9236(2) & 19(1) \\ C(13) & 10968(1) & 6187(1) & 8965(2) & 21(1) \\ C(14) & 11217(1) & 6479(1) & 9465(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10223(2) & 16(1) \\ C(16) & 11289(1) & 6861(1) & 10797(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(21) & 10905(1) & 7130(1) & 12784(2) & 20(1) \\ C(22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7302(1) & 14106(2) & 34(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 11204(1) & 6063(1) & 13519(2) & 26(1) \\ C(30) & 10688(1) & 5365(1) & 14687(2) & 43(1) \\ C(30) & 10688(1) & 5345(1) & 114249(2) & 41(1) \\ C(31) & 10668(1) & 5416(1) & 13441(2) & 30(1) \\ C(32) & 11447(1) & 5772(1) & 11614(2) & 18(1) \\ C(33) & 11816(1) & 6081(1) & 1793(2) & 23(1) \\ C(34) & 12250(1) & 6035(1) & 114249(2) & 41(1) \\ C(35) & 12335(1) & 5661(1) & 10922(2) & 40(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5413(1) & 11079(2) & 28(1) \\ N(1) & 10084(1) & 7125(1) & 11268(1) & 17(1) \\ N(2) & 9779(1) & 6281(1) & 11704(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 14486(1) & 14(1) \\ N(4) & 11067(1) & 6868(1) & 12716(1) & 18(1) \\ O(1) & 10594(1) & 7375(1) & 17605(1) & 28(1) \\ F(1) & 12430(1) & 7375(1) & 17605(1) & 28(1) \\ F(1) & 12430(1) & 7375(1) & 17605(1) & 28(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(5) & 11668(1) & 7145(1) & 17720(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17735(1) & 23(1) \\ F(4) & 12266(1) & 6888(1) & 17735(1) & 23(1) \\ F(4) & 1224(1) & 6808(1) & 17735(1) & 23(1) \\ F(4) & 1224(1) & 6008(1) & 14232(2) & 35(1) \\ F(2) & 1224(1) & 6008(1) & 14232(2) & 35(1) \\ F(2) & 10000 & 5000 & 10634(2) & 25(1) \\ \hline \end{array}$	C(10)	9631(1)	5843(1)	11870(2)	17(1)
$\begin{array}{ccccc} C(12) & 10567(1) & 5966(1) & 9236(2) & 19(1) \\ C(13) & 10968(1) & 6187(1) & 8965(2) & 21(1) \\ C(14) & 11217(1) & 6479(1) & 9465(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10223(2) & 16(1) \\ C(16) & 11289(1) & 6861(1) & 10797(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 110673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(21) & 10905(1) & 7130(1) & 12784(2) & 20(1) \\ C(22) & 10905(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7302(1) & 14106(2) & 34(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 11204(1) & 6063(1) & 13519(2) & 26(1) \\ C(29) & 10964(1) & 5663(1) & 14687(2) & 43(1) \\ C(31) & 10668(1) & 53416(1) & 13441(2) & 30(1) \\ C(32) & 11447(1) & 5772(1) & 11614(2) & 18(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(34) & 12250(1) & 6035(1) & 114444(2) & 31(1) \\ C(35) & 12335(1) & 5681(1) & 10922(2) & 40(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5413(1) & 11079(2) & 28(1) \\ N(1) & 10084(1) & 7125(1) & 11268(1) & 17(1) \\ N(2) & 9779(1) & 6281(1) & 11793(2) & 23(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5413(1) & 11079(2) & 28(1) \\ N(1) & 10084(1) & 7125(1) & 11268(1) & 17(1) \\ N(2) & 9779(1) & 6281(1) & 17746(1) & 23(1) \\ F(1) & 1230(1) & 6330(1) & 12716(1) & 18(1) \\ O(1) & 10594(1) & 7375(1) & 17605(1) & 28(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 1266(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 1266(1) & 6624(1) & 17735(1) & 23(1) \\ F(4) & 1266(1) & 6624(1) & 17735(1) & 23(1) \\ F(4) & 1266(1) & 6624(1) & 17735(1) & 23(1) \\ F(4) & 1266(1) & 6624(1) & 17735(1) & 23(1) \\ F(4) & 1266(1) & 6624(1) & 17735(1) & 23(1) \\ F(4) & 10481(1) & 521(1) & 11625(1) & 14(1) \\ C(28) & 11224(1) & 6008(1) & 14323(2) & 35(1) \\ C(2) & 10000 & 5000 & 10634(2) & 25(1) \\ \end{array}$	C(11)	10421(1)	6048(1)	9997(2)	18(1)
$\begin{array}{cccccc} C(13) & 10968(1) & 6187(1) & 8965(2) & 21(1) \\ C(14) & 11217(1) & 6479(1) & 9465(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10223(2) & 16(1) \\ C(16) & 11289(1) & 6861(1) & 10797(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(19) & 11596(1) & 7149(1) & 12091(2) & 19(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(21) & 10905(1) & 7367(1) & 13479(2) & 28(1) \\ C(22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7302(1) & 14106(2) & 34(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 11204(1) & 6063(1) & 13519(2) & 26(1) \\ C(29) & 10964(1) & 5365(1) & 14249(2) & 41(1) \\ C(30) & 10688(1) & 5365(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5416(1) & 13441(2) & 18(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(34) & 12250(1) & 635(1) & 114444(2) & 18(1) \\ C(35) & 12335(1) & 5681(1) & 10922(2) & 40(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5413(1) & 11079(2) & 28(1) \\ N(1) & 10084(1) & 7125(1) & 11268(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 10488(1) & 14(1) \\ N(4) & 11067(1) & 688(1) & 11499(1) & 16(1) \\ N(5) & 10530(1) & 6336(1) & 10488(1) & 14(1) \\ N(4) & 10067(1) & 688(1) & 11774(1) & 23(1) \\ F(1) & 12430(1) & 7375(1) & 127605(1) & 28(1) \\ F(1) & 12430(1) & 7375(1) & 177605(1) & 28(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 1224(1) & 6088(1) & 17735(1) & 23(1) \\ Ru(1) & 10481(1) & 6521(1) & 11625(1) & 14(1) \\ C(28) & 11224(1) & 6000 & 10634(2) & 25$	C(12)	10567(1)	5966(1)	9236(2)	19(1)
$\begin{array}{ccccc} C(14) & 11217(1) & 6479(1) & 9465(2) & 20(1) \\ C(15) & 11056(1) & 6551(1) & 10223(2) & 16(1) \\ C(16) & 11289(1) & 6861(1) & 10797(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(20) & 11205(1) & 7149(1) & 12091(2) & 19(1) \\ C(21) & 10905(1) & 7130(1) & 12784(2) & 26(1) \\ C(22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7302(1) & 14106(2) & 34(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 11204(1) & 6063(1) & 13519(2) & 26(1) \\ C(29) & 10964(1) & 5663(1) & 14249(2) & 41(1) \\ C(30) & 10688(1) & 5345(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5345(1) & 11444(2) & 30(1) \\ C(32) & 11447(1) & 5772(1) & 11614(2) & 18(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(34) & 12250(1) & 6035(1) & 11444(2) & 31(1) \\ C(35) & 12335(1) & 5661(1) & 10922(2) & 40(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5413(1) & 11079(2) & 28(1) \\ N(1) & 10084(1) & 7125(1) & 11268(1) & 17(1) \\ N(2) & 9779(1) & 6281(1) & 11794(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 10488(1) & 14(1) \\ N(4) & 11067(1) & 6880(1) & 12716(1) & 18(1) \\ O(1) & 10594(1) & 5376(1) & 11744(1) & 23(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(5) & 11668(1) & 7145(1) & 17720(1) & 35(1) \\ F(6) & 12134(1) & 6322(1) & 17860(1) & 42(1) \\ F(4) & 12666(1) & 6139(1) & 17745(1) & 35(1) \\ F(5) & 11668(1) & 7145(1) & 17720(1) & 35(1) \\ F(6) & 12134(1) & 6322(1) & 17860(1) & 27(1) \\ P(1) & 10844(1) & 5822(1) & 11999(1) & 16(1) \\ P(2) & 12166(1) & 688(1) & 17735(1) & 23(1) \\ F(4) & 1224(1) & 6008(1) & 17735(1) & 23(1) \\ F(4) & 10644(1) & 5822(1) & 11999(1) & 16(1) \\ P(2) & 12166(1) & 688(1) & 17735(1) & 23(1) \\ F(4) & 10641(1) & 6521(1) & 11625(1) & 14(1) \\ O(2) & 10000 & 5000 & 10634(2) & 25(1) \\ \end{array}$	C(13)	10968(1)	6187(1)	8965(2)	21(1)
$\begin{array}{ccccc} C(15) & 11056(1) & 6551(1) & 10223(2) & 16(1) \\ C(16) & 11289(1) & 6851(1) & 10797(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(21) & 10905(1) & 7130(1) & 12784(2) & 20(1) \\ C(22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7032(1) & 14106(2) & 34(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(29) & 10964(1) & 5663(1) & 14687(2) & 43(1) \\ C(30) & 10688(1) & 5365(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5416(1) & 13414(2) & 30(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(36) & 11250(1) & 6035(1) & 11644(2) & 18(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 51369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5136(1) & 10922(2) & 40(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5136(1) & 10948(1) & 17(1) \\ N(1) & 10084(1) & 7125(1) & 11268(1) & 17(1) \\ N(2) & 9779(1) & 6281(1) & 11741(1) & 23(1) \\ F(1) & 1230(1) & 6336(1) & 10488(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 10748(1) & 14(1) \\ N(4) & 11067(1) & 6868(1) & 11741(1) & 23(1) \\ F(4) & 12666(1) & 624(1) & 17745(1) & 35(1) \\ F(5) & 11668(1) & 7145(1) & 177605(1) & 28(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(5) & 11668(1) & 7145(1) & 17720(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12266(1) & 688(1) & 17735(1) & 23(1) \\ F(4) & 12266(1) & 688(1) & 17735(1) & 23(1) \\ F(4) & 12266(1) & 688(1) & 17735(1) & 23(1) \\ F(4) & 1224(1) & 6008(1) & 14222(2) & 35(1) \\ O(2) & 10000 & 5000 & 10634(2) & 25(1) \\ \end{array}$	C(14)	11217(1)	6479(1)	9465(2)	20(1)
$\begin{array}{cccc} C(16) & 11229(1) & 6861(1) & 10(97(2) & 18(1) \\ C(17) & 11681(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(19) & 11596(1) & 7444(1) & 11982(2) & 26(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(21) & 10905(1) & 7130(1) & 12784(2) & 20(1) \\ C(22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7302(1) & 14106(2) & 34(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 11204(1) & 6063(1) & 13519(2) & 26(1) \\ C(29) & 10964(1) & 5663(1) & 14249(2) & 41(1) \\ C(30) & 10688(1) & 5345(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5416(1) & 13441(2) & 30(1) \\ C(32) & 11447(1) & 5772(1) & 11614(2) & 18(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(34) & 12250(1) & 6035(1) & 11444(2) & 31(1) \\ C(35) & 12335(1) & 5681(1) & 10092(2) & 40(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5413(1) & 11079(2) & 28(1) \\ N(1) & 10084(1) & 7125(1) & 11268(1) & 17(1) \\ N(2) & 9779(1) & 6281(1) & 11704(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 10488(1) & 14(1) \\ N(4) & 11067(1) & 6866(1) & 11499(1) & 16(1) \\ N(3) & 10651(1) & 633(1) & 12716(1) & 18(1) \\ O(1) & 10594(1) & 7376(1) & 11741(1) & 23(1) \\ F(4) & 12666(1) & 6224(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 632(1) & 17735(1) & 28(1) \\ F(2) & 12192(1) & 6953(1) & 18662(1) & 44(1) \\ F(3) & 11903(1) & 6392(1) & 17860(1) & 42(1) \\ F(4) & 12666(1) & 6144(1) & 16080(1) & 27(1) \\ P(1) & 10844(1) & 5822(1) & 11999(1) & 16(1) \\ P(2) & 1216(1) & 688(1) & 17735(1) & 23(1) \\ F(4) & 12260(1) & 6822(1) & 11999(1) & 16(1) \\ P(2) & 1216(1) & 688(1) & 17735(1) & 23(1) \\ F(4) & 1226(1) & 688(1) & 17735(1) & 23(1) \\ F(4) & 1226(1) & 688(1) & 17735(1) & 23(1) \\ F(4) & 1226(1) & 608(1) & 14323(2) & 35(1) \\ F(2) & 12124(1) & 6008(1) & 14323(2) & 35(1) \\ F(2) & 1224(1) & 6008(1) & 14323(2) & 35(1) \\ F(2) & 10000 & 5000 & 10634(2) & 25(1) \\ \end{array} \right)$	C(15)	11056(1)	6551(1)	10223(2)	16(1)
$\begin{array}{cccccc} C(17) & 11661(1) & 7142(1) & 10673(2) & 25(1) \\ C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(21) & 10905(1) & 7130(1) & 12784(2) & 20(1) \\ C(22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7302(1) & 14106(2) & 34(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 11204(1) & 6063(1) & 13519(2) & 26(1) \\ C(29) & 10964(1) & 5665(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5416(1) & 13441(2) & 30(1) \\ C(32) & 11447(1) & 5772(1) & 11614(2) & 18(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(34) & 12250(1) & 56681(1) & 10922(2) & 40(1) \\ C(35) & 12335(1) & 5681(1) & 10922(2) & 40(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5143(1) & 11079(2) & 28(1) \\ N(1) & 10084(1) & 7125(1) & 11268(1) & 17(1) \\ N(2) & 9779(1) & 6281(1) & 11704(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 10488(1) & 14(1) \\ N(4) & 11067(1) & 688(1) & 11749(1) & 14(1) \\ N(4) & 11067(1) & 6830(1) & 12716(1) & 18(1) \\ O(11) & 10594(1) & 7376(1) & 11741(1) & 23(1) \\ F(2) & 12192(1) & 6935(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17735(1) & 27(1) \\ P(1) & 10844(1) & 5822(1) & 11999(1) & 16(1) \\ P(2) & 1216(1) & 6814(1) & 1625(1) & 14(1) \\ P(2) & 1216(1) & 6814(1) & 14223(2) & 35(1) \\ P(2) & 1216(1) & 6814(1) & 1625(1) & 14(1) \\ P(2) & 1216(1) & 6818(1) & 17735(1) & 23(1) \\ P(2) & 1216(1) & 6818(1) & 17735(1) & 23(1) \\ P(2) & 1226(1) & 6818(1) & 17735(1) & 23(1) \\ P(2) & 1226(1) & 6818(1) & 17735(1) & 23(1) \\ P(2) & 1226(1) & 6818(1) & 17735(1) & 23(1) \\ P(2) & 1226(1) & 6088(1) & 17735(1) & 23(1) \\ P(2) & 1226(1) & 6088(1) & 17735(1) & 23(1) \\ P(2) & 1226(1) & 6008(1) & 14223(2) & 35(1) \\ P(2) & 10000 & 5000 & 10634(2) & 25(1) \\ \end{array} \right)$	C(16)	11289(1)	6861(1) 5140(1)	10/9/(2)	18(1)
$\begin{array}{cccc} C(18) & 11837(1) & 7429(1) & 11277(2) & 29(1) \\ C(19) & 11596(1) & 7444(1) & 11982(2) & 26(1) \\ C(20) & 11205(1) & 7159(1) & 12091(2) & 19(1) \\ C(21) & 10905(1) & 7130(1) & 12784(2) & 20(1) \\ C(22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ C(23) & 10695(1) & 7302(1) & 14006(2) & 34(1) \\ C(24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 11204(1) & 6063(1) & 13519(2) & 26(1) \\ C(29) & 10964(1) & 5663(1) & 14687(2) & 43(1) \\ C(30) & 10688(1) & 5365(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5416(1) & 13441(2) & 30(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(34) & 12250(1) & 6035(1) & 11444(2) & 31(1) \\ C(35) & 12335(1) & 5681(1) & 10922(2) & 40(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ N(1) & 10084(1) & 7125(1) & 11268(1) & 17(1) \\ N(2) & 9779(1) & 6281(1) & 11794(1) & 14(1) \\ N(4) & 11067(1) & 688(1) & 11499(1) & 16(1) \\ N(4) & 1067(1) & 6336(1) & 1148(1) & 144(1) \\ N(4) & 1067(1) & 6336(1) & 11741(1) & 23(1) \\ F(1) & 12430(1) & 7375(1) & 17605(1) & 28(1) \\ F(2) & 12192(1) & 6953(1) & 18662(1) & 44(1) \\ F(3) & 11903(1) & 6392(1) & 1778(1) & 35(1) \\ F(4) & 12666(1) & 7145(1) & 17720(1) & 35(1) \\ F(4) & 12666(1) & 7145(1) & 17720(1) & 35(1) \\ F(4) & 12666(1) & 7145(1) & 17735(1) & 27(1) \\ P(1) & 10844(1) & 5822(1) & 11999(1) & 16(1) \\ P(2) & 12166(1) & 6088(1) & 17735(1) & 27(1) \\ P(1) & 10844(1) & 5822(1) & 11999(1) & 16(1) \\ P(2) & 12166(1) & 6088(1) & 17735(1) & 23(1) \\ Ru(1) & 10481(1) & 6521(1) & 14323(2) & 35(1) \\ P(2) & 1224(1) & 6008(1) & 14323(2) & 35(1) \\ P(2) & 1224(1) & 6008(1) & 14323(2) & 35(1) \\ P(2) & 10000 & 5000 & 10634(2) & 25(1) \\ \end{array} \right)$	C(1/)	11681(1)	7142(1)	106/3(2)	25(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(18)	1183/(1) 1150C(1)	7429(1)	112//(2)	29(1)
$\begin{array}{ccccccc} (20) & 11203(1) & 1239(1) & 1203(2) & 19(1) \\ (21) & 10905(1) & 7130(1) & 12784(2) & 20(1) \\ (22) & 10988(1) & 7367(1) & 13479(2) & 28(1) \\ (23) & 10695(1) & 7302(1) & 14106(2) & 34(1) \\ (24) & 10320(1) & 7003(1) & 14039(2) & 31(1) \\ (25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ (26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ (27) & 11204(1) & 6063(1) & 13519(2) & 26(1) \\ (29) & 10964(1) & 5365(1) & 14269(2) & 41(1) \\ (30) & 10688(1) & 5365(1) & 14249(2) & 41(1) \\ (31) & 10668(1) & 5416(1) & 13441(2) & 30(1) \\ (32) & 11447(1) & 5772(1) & 11614(2) & 18(1) \\ (33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ (34) & 12250(1) & 6035(1) & 11444(2) & 31(1) \\ (35) & 12335(1) & 5681(1) & 10737(2) & 42(1) \\ (37) & 11534(1) & 5369(1) & 10737(2) & 42(1) \\ (37) & 11534(1) & 5413(1) & 11079(2) & 28(1) \\ N(1) & 10084(1) & 7125(1) & 11268(1) & 17(1) \\ N(2) & 9779(1) & 6281(1) & 11704(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 10488(1) & 14(1) \\ N(4) & 11067(1) & 6868(1) & 11499(1) & 16(1) \\ N(5) & 10530(1) & 6330(1) & 12716(1) & 18(1) \\ 0(1) & 10594(1) & 5376(1) & 11741(1) & 23(1) \\ F(1) & 12430(1) & 7375(1) & 17605(1) & 28(1) \\ F(2) & 12192(1) & 6953(1) & 18662(1) & 44(1) \\ F(3) & 11903(1) & 6322(1) & 17860(1) & 42(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(6) & 12134(1) & 6814(1) & 16806(1) & 27(1) \\ P(1) & 10844(1) & 5822(1) & 11999(1) & 16(1) \\ P(2) & 12166(1) & 688(1) & 17735(1) & 23(1) \\ F(4) & 1266(1) & 688(1) & 17735(1) & 23(1) \\ F(4) & 10641(1) & 6521(1) & 11625(1) & 14(1) \\ P(2) & 12166(1) & 6808(1) & 17735(1) & 23(1) \\ F(2) & 11224(1) & 6008(1) & 14323(2) & 35(1) \\ O(2) & 10000 & 5000 & 10634(2) & 25(1) \\ \end{array}$	C(19)	11205(1)	7444(L) 7150(1)	11982(2)	20(1) 10(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(20)	11205(1)	7139(1)	12091(2) 12784(2)	19(1)
$\begin{array}{ccccccc} C(22) & 10000(1) & 13070(1) & 13479(2) & 26(1) \\ C(23) & 10095(1) & 7003(1) & 1409(2) & 31(1) \\ C(25) & 10245(1) & 6771(1) & 13341(2) & 23(1) \\ C(26) & 10925(1) & 5766(1) & 13064(2) & 19(1) \\ C(27) & 11204(1) & 6063(1) & 13519(2) & 26(1) \\ C(29) & 10964(1) & 5663(1) & 14687(2) & 43(1) \\ C(30) & 10688(1) & 5365(1) & 14249(2) & 41(1) \\ C(31) & 10668(1) & 5416(1) & 13441(2) & 30(1) \\ C(32) & 11447(1) & 5772(1) & 11614(2) & 18(1) \\ C(33) & 11816(1) & 6081(1) & 11793(2) & 23(1) \\ C(34) & 12250(1) & 6035(1) & 11444(2) & 31(1) \\ C(35) & 12335(1) & 5681(1) & 10922(2) & 40(1) \\ C(36) & 11978(1) & 5369(1) & 10737(2) & 42(1) \\ C(37) & 11534(1) & 5413(1) & 11079(2) & 28(1) \\ N(1) & 10084(1) & 7125(1) & 11268(1) & 17(1) \\ N(2) & 9779(1) & 6281(1) & 11704(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 10488(1) & 14(1) \\ N(3) & 10651(1) & 6336(1) & 10488(1) & 14(1) \\ N(4) & 11067(1) & 6868(1) & 11499(1) & 16(1) \\ N(5) & 10530(1) & 6830(1) & 12716(1) & 18(1) \\ O(1) & 10594(1) & 5376(1) & 11741(1) & 23(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6624(1) & 17745(1) & 35(1) \\ F(4) & 12666(1) & 6888(1) & 17735(1) & 23(1) \\ F(4) & 12666(1) & 6888(1) & 17735(1) & 23(1) \\ F(4) & 10844(1) & 5822(1) & 11999(1) & 16(1) \\ P(2) & 12166(1) & 6888(1) & 17735(1) & 23(1) \\ F(4) & 100481(1) & 6521(1) & 11625(1) & 14(1) \\ C(28) & 11224(1) & 6008(1) & 14323(2) & 35(1) \\ O(2) & 10000 & 5000 & 10634(2) & 25(1) \\ \end{array} \right)$	C(21)	10905(1)	7367(1)	13/79(2)	20(1)
C (24)10320 (1)7003 (1)1110 (2)31 (1)C (25)10245 (1)6771 (1)13341 (2)23 (1)C (26)10925 (1)5766 (1)13064 (2)19 (1)C (27)11204 (1)6063 (1)13519 (2)26 (1)C (29)10964 (1)5663 (1)14687 (2)43 (1)C (30)10688 (1)5365 (1)14249 (2)41 (1)C (31)10668 (1)5416 (1)13441 (2)30 (1)C (32)11447 (1)5772 (1)11614 (2)18 (1)C (33)11816 (1)6035 (1)11444 (2)31 (1)C (34)12250 (1)6035 (1)11444 (2)31 (1)C (36)11978 (1)5369 (1)10737 (2)42 (1)C (37)11534 (1)5413 (1)11079 (2)28 (1)N (1)10084 (1)7125 (1)11268 (1)17 (1)N (2)9779 (1)6281 (1)10748 (1)14 (1)N (3)10651 (1)6336 (1)10488 (1)14 (1)N (4)11067 (1)6868 (1)11499 (1)16 (1)N (5)10530 (1)6330 (1)12716 (1)18 (1)O (1)10594 (1)5376 (1)11745 (1)35 (1)F (4)12666 (1)6624 (1)17745 (1)35 (1)F (5)11668 (1)7145 (1)17720 (1)35 (1)F (6)12134 (1)6814 (1)16806 (1)27 (1)F (6)12134 (1)6088 (1)17735 (1)23 (1)F (6)121	C(22)	10695(1)	7302(1)	13479(2) 14106(2)	20(1) 34(1)
C (21)10245 (1)700 (1)110341 (2)23 (1)C (26)10925 (1)5766 (1)13341 (2)23 (1)C (27)11204 (1)6063 (1)13519 (2)26 (1)C (29)10964 (1)5663 (1)14687 (2)43 (1)C (30)10688 (1)5365 (1)14249 (2)41 (1)C (31)10668 (1)5416 (1)13441 (2)30 (1)C (32)11447 (1)5772 (1)11614 (2)18 (1)C (33)11816 (1)6081 (1)11793 (2)23 (1)C (34)12250 (1)6035 (1)11444 (2)31 (1)C (36)11978 (1)5369 (1)10737 (2)42 (1)C (37)11534 (1)5413 (1)11079 (2)28 (1)N (1)10084 (1)7125 (1)11268 (1)17 (1)N (2)9779 (1)6281 (1)11704 (1)14 (1)N (3)10651 (1)6336 (1)10488 (1)14 (1)N (4)11067 (1)6868 (1)11499 (1)16 (1)N (5)10530 (1)6330 (1)12716 (1)18 (1)O (1)10594 (1)5376 (1)11745 (1)23 (1)F (2)12192 (1)6953 (1)18662 (1)44 (1)F (3)11903 (1)6392 (1)17860 (1)42 (1)F (4)12666 (1)6624 (1)17745 (1)35 (1)F (5)11668 (1)7145 (1)17720 (1)35 (1)F (6)12134 (1)6814 (1)16606 (1)27 (1)P (1)108	C(23)	10000(1) 10320(1)	7003(1)	14039(2)	31(1)
C (26)10925(1)5766(1)13064(2)19(1)C (27)11204(1)6063(1)13519(2)26(1)C (29)10964(1)5663(1)14687(2)43(1)C (30)10688(1)5365(1)14249(2)41(1)C (31)10668(1)5416(1)13441(2)30(1)C (32)11447(1)5772(1)11614(2)18(1)C (33)11816(1)6081(1)11793(2)23(1)C (34)12250(1)6035(1)11444(2)31(1)C (36)11978(1)5369(1)10737(2)42(1)C (37)11534(1)5413(1)11079(2)28(1)N (1)10084(1)7125(1)11268(1)17(1)N (2)9779(1)6281(1)11704(1)14(1)N (3)10651(1)6336(1)10488(1)14(1)N (4)11067(1)6880(1)11499(1)16(1)N (5)10530(1)6330(1)12716(1)18(1)O (1)10594(1)5376(1)117605(1)28(1)F (2)12192(1)6953(1)18662(1)44(1)F (3)11903(1)6392(1)17860(1)42(1)F (4)12666(1)6624(1)17735(1)35(1)F (6)12134(1)6814(1)1680(1)27(1)P (1)10844(1)5822(1)11999(1)16(1)P (1)10481(1)6521(1)14323(2)35(1)C (2)10000500010634(2)25(1)	C(25)	10245(1)	6771(1)	13341(2)	23(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(26)	10925(1)	5766(1)	13064(2)	19(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(27)	11204(1)	6063(1)	13519(2)	26(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(29)	10964(1)	5663(1)	14687(2)	43(1)
C (31)10668 (1) $5416(1)$ 13441 (2) $30(1)$ C (32)11447 (1) $5772(1)$ 11614 (2)18 (1)C (33)11816 (1) $6081(1)$ 11793 (2)23 (1)C (34)12250 (1) $6035(1)$ 11444 (2)31 (1)C (35)12335 (1) $5681(1)$ 10922 (2)40 (1)C (36)11978 (1) $5369(1)$ 10737 (2)42 (1)C (37)11534 (1) $5413(1)$ 11079 (2)28 (1)N (1)10084 (1)7125 (1)11268 (1)17 (1)N (2)9779 (1)6281 (1)11704 (1)14 (1)N (3)10651 (1)6336 (1)10488 (1)14 (1)N (4)11067 (1)6868 (1)11499 (1)16 (1)N (5)10530 (1)6830 (1)12716 (1)18 (1)O (1)10594 (1)5376 (1)117605 (1)28 (1)F (1)12430 (1)7375 (1)17605 (1)28 (1)F (2)12192 (1)6953 (1)18662 (1)44 (1)F (3)11903 (1)6392 (1)17860 (1)42 (1)F (4)12666 (1)6624 (1)17745 (1)35 (1)F (5)11668 (1)7145 (1)16806 (1)27 (1)P (1)10844 (1)5822 (1)11999 (1)16 (1)P (2)12166 (1)6888 (1)17735 (1)23 (1)Ru (1)10481 (1)6521 (1)14323 (2)35 (1)O (2)10000500010634 (2)25 (1)	C(30)	10688(1)	5365(1)	14249(2)	41(1)
C (32)11447 (1) $5772 (1)$ 11614 (2)18 (1)C (33)11816 (1)6081 (1)11793 (2)23 (1)C (34)12250 (1)6035 (1)11444 (2)31 (1)C (35)12335 (1)5681 (1)10922 (2)40 (1)C (36)11978 (1)5369 (1)10737 (2)42 (1)C (37)11534 (1)5413 (1)11079 (2)28 (1)N (1)10084 (1)7125 (1)11268 (1)17 (1)N (2)9779 (1)6281 (1)11704 (1)14 (1)N (3)10651 (1)6336 (1)10488 (1)14 (1)N (4)11067 (1)6868 (1)11499 (1)16 (1)N (5)10530 (1)6830 (1)12716 (1)18 (1)O (1)10594 (1)5376 (1)11741 (1)23 (1)F (1)12430 (1)7375 (1)17605 (1)28 (1)F (2)12192 (1)6953 (1)18662 (1)44 (1)F (3)11903 (1)6392 (1)17860 (1)42 (1)F (4)12666 (1)6624 (1)17745 (1)35 (1)F (6)12134 (1)6814 (1)16806 (1)27 (1)P (1)10844 (1)5822 (1)11999 (1)16 (1)P (2)12166 (1)688 (1)17735 (1)23 (1)Ru (1)10481 (1)6521 (1)14323 (2)35 (1)O (2)10000500010634 (2)25 (1)	C(31)	10668(1)	5416(1)	13441(2)	30(1)
C (33)11816(1) $6081(1)$ $11793(2)$ $23(1)$ C (34)12250(1) $6035(1)$ $11444(2)$ $31(1)$ C (35)12335(1) $5681(1)$ $10922(2)$ $40(1)$ C (36) $11978(1)$ $5369(1)$ $10737(2)$ $42(1)$ C (37) $11534(1)$ $5413(1)$ $11079(2)$ $28(1)$ N (1) $10084(1)$ $7125(1)$ $11268(1)$ $17(1)$ N (2) $9779(1)$ $6281(1)$ $11704(1)$ $14(1)$ N (3) $10651(1)$ $6336(1)$ $10488(1)$ $14(1)$ N (4) $11067(1)$ $6868(1)$ $11499(1)$ $16(1)$ N (5) $10530(1)$ $6830(1)$ $12716(1)$ $18(1)$ O (1) $10594(1)$ $5376(1)$ $1745(1)$ $28(1)$ F (1) $12430(1)$ $7375(1)$ $17605(1)$ $28(1)$ F (3) $11903(1)$ $6392(1)$ $17860(1)$ $42(1)$ F (4) $12666(1)$ $6624(1)$ $17745(1)$ $35(1)$ F (5) $11668(1)$ $7145(1)$ $17720(1)$ $35(1)$ F (6) $12134(1)$ $6814(1)$ $16806(1)$ $27(1)$ P (1) $10844(1)$ $5822(1)$ $11999(1)$ $16(1)$ P (2) $12166(1)$ $688(1)$ $17735(1)$ $23(1)$ Ru (1) $10481(1)$ $6521(1)$ $14323(2)$ $35(1)$ O (2) $10000$ $5000$ $10634(2)$ $25(1)$	C(32)	11447(1)	5772(1)	11614(2)	18(1)
C (34)12250(1) $6035(1)$ 11444(2) $31(1)$ C (35)12335(1) $5681(1)$ $10922(2)$ $40(1)$ C (36)11978(1) $5369(1)$ $10737(2)$ $42(1)$ C (37)11534(1) $5413(1)$ $11079(2)$ $28(1)$ N (1)10084(1) $7125(1)$ $11268(1)$ $17(1)$ N (2) $9779(1)$ $6281(1)$ $11704(1)$ $14(1)$ N (3) $10651(1)$ $6336(1)$ $10488(1)$ $14(1)$ N (4) $11067(1)$ $6868(1)$ $11499(1)$ $16(1)$ N (5) $10530(1)$ $6830(1)$ $12716(1)$ $18(1)$ O (1) $10594(1)$ $5376(1)$ $11741(1)$ $23(1)$ F (1) $12430(1)$ $7375(1)$ $17605(1)$ $28(1)$ F (2) $12192(1)$ $6953(1)$ $18662(1)$ $44(1)$ F (3) $11903(1)$ $6392(1)$ $17860(1)$ $42(1)$ F (4) $12666(1)$ $6624(1)$ $17745(1)$ $35(1)$ F (6) $12134(1)$ $6814(1)$ $16806(1)$ $27(1)$ F (6) $12134(1)$ $6814(1)$ $17735(1)$ $23(1)$ Ru (1) $10481(1)$ $6521(1)$ $14323(2)$ $35(1)$ Ru (1) $10481(1)$ $6008(1)$ $14323(2)$ $35(1)$ O (2) $10000$ $5000$ $10634(2)$ $25(1)$	C(33)	11816(1)	6081(1)	11793(2)	23(1)
C (35)12335(1) $5681(1)$ $10922(2)$ $40(1)$ C (36)11978(1) $5369(1)$ $10737(2)$ $42(1)$ C (37)11534(1) $5413(1)$ $11079(2)$ $28(1)$ N (1) $10084(1)$ $7125(1)$ $11268(1)$ $17(1)$ N (2) $9779(1)$ $6281(1)$ $11704(1)$ $14(1)$ N (3) $10651(1)$ $6336(1)$ $10488(1)$ $14(1)$ N (4) $11067(1)$ $6868(1)$ $11499(1)$ $16(1)$ N (5) $10530(1)$ $6830(1)$ $12716(1)$ $18(1)$ O (1) $10594(1)$ $5376(1)$ $11741(1)$ $23(1)$ F (1) $12430(1)$ $7375(1)$ $17605(1)$ $28(1)$ F (2) $12192(1)$ $6953(1)$ $18662(1)$ $44(1)$ F (3) $11903(1)$ $6392(1)$ $17860(1)$ $42(1)$ F (4) $12666(1)$ $6624(1)$ $17745(1)$ $35(1)$ F (6) $12134(1)$ $6814(1)$ $16806(1)$ $27(1)$ P (1) $10844(1)$ $5822(1)$ $11999(1)$ $16(1)$ P (2) $12166(1)$ $688(1)$ $17735(1)$ $23(1)$ Ru (1) $10481(1)$ $6521(1)$ $14323(2)$ $35(1)$ O (2) $10000$ $5000$ $10634(2)$ $25(1)$	C(34)	12250(1)	6035(1)	11444(2)	31(1)
C (36) $11978(1)$ $5369(1)$ $10737(2)$ $42(1)$ C (37) $11534(1)$ $5413(1)$ $11079(2)$ $28(1)$ N (1) $10084(1)$ $7125(1)$ $11268(1)$ $17(1)$ N (2) $9779(1)$ $6281(1)$ $11704(1)$ $14(1)$ N (3) $10651(1)$ $6336(1)$ $10488(1)$ $14(1)$ N (4) $11067(1)$ $6868(1)$ $11499(1)$ $16(1)$ N (5) $10530(1)$ $6830(1)$ $12716(1)$ $18(1)$ O (1) $10594(1)$ $5376(1)$ $11741(1)$ $23(1)$ F (1) $12430(1)$ $7375(1)$ $17605(1)$ $28(1)$ F (2) $12192(1)$ $6953(1)$ $18662(1)$ $44(1)$ F (3) $11903(1)$ $6392(1)$ $17745(1)$ $35(1)$ F (4) $12666(1)$ $6624(1)$ $17745(1)$ $35(1)$ F (6) $12134(1)$ $6814(1)$ $16806(1)$ $27(1)$ P (1) $10844(1)$ $5822(1)$ $11999(1)$ $16(1)$ P (2) $12166(1)$ $621(1)$ $17735(1)$ $23(1)$ Ru (1) $10481(1)$ $6521(1)$ $14323(2)$ $35(1)$ O (2) $10000$ $5000$ $10634(2)$ $25(1)$	C(35)	12335(1)	5681(1)	10922(2)	40(1)
C $(37)$ 11534 (1)5413 (1)11079 (2)28 (1)N (1)10084 (1)7125 (1)11268 (1)17 (1)N (2)9779 (1)6281 (1)11704 (1)14 (1)N (3)10651 (1)6336 (1)10488 (1)14 (1)N (4)11067 (1)6868 (1)11499 (1)16 (1)N (5)10530 (1)6830 (1)12716 (1)18 (1)O (1)10594 (1)5376 (1)11741 (1)23 (1)F (1)12430 (1)7375 (1)17605 (1)28 (1)F (2)12192 (1)6953 (1)18662 (1)44 (1)F (3)11903 (1)6392 (1)17860 (1)42 (1)F (4)12666 (1)6624 (1)17745 (1)35 (1)F (5)11668 (1)7145 (1)17720 (1)35 (1)F (6)12134 (1)6814 (1)16806 (1)27 (1)P (1)10844 (1)5822 (1)11999 (1)16 (1)P (2)12166 (1)6521 (1)11625 (1)14 (1)C (28)11224 (1)6008 (1)14323 (2)35 (1)O (2)10000500010634 (2)25 (1)	C(36)	11978(1)	5369(1)	10737(2)	42(1)
N (1) $10084(1)$ $7125(1)$ $11268(1)$ $17(1)$ N(2) $9779(1)$ $6281(1)$ $11704(1)$ $14(1)$ N(3) $10651(1)$ $6336(1)$ $10488(1)$ $14(1)$ N(4) $11067(1)$ $6868(1)$ $11499(1)$ $16(1)$ N(5) $10530(1)$ $6830(1)$ $12716(1)$ $18(1)$ O(1) $10594(1)$ $5376(1)$ $11741(1)$ $23(1)$ F(1) $12430(1)$ $7375(1)$ $17605(1)$ $28(1)$ F(2) $12192(1)$ $6953(1)$ $18662(1)$ $44(1)$ F(3) $11903(1)$ $6392(1)$ $17860(1)$ $42(1)$ F(4) $12666(1)$ $6624(1)$ $17745(1)$ $35(1)$ F(5) $11668(1)$ $7145(1)$ $17720(1)$ $35(1)$ F(6) $12134(1)$ $6814(1)$ $16806(1)$ $27(1)$ P(1) $10844(1)$ $5822(1)$ $11999(1)$ $16(1)$ P(2) $12166(1)$ $6888(1)$ $17735(1)$ $23(1)$ Ru(1) $10481(1)$ $6521(1)$ $14323(2)$ $35(1)$ O(2) $10000$ $5000$ $10634(2)$ $25(1)$	C(37)	11534(1)	5413(1)	11079(2)	28(1)
N (2) $9779(1)$ $6281(1)$ $11704(1)$ $14(1)$ N (3) $10651(1)$ $6336(1)$ $10488(1)$ $14(1)$ N (4) $11067(1)$ $6868(1)$ $11499(1)$ $16(1)$ N (5) $10530(1)$ $6830(1)$ $12716(1)$ $18(1)$ O (1) $10594(1)$ $5376(1)$ $11741(1)$ $23(1)$ F (1) $12430(1)$ $7375(1)$ $17605(1)$ $28(1)$ F (2) $12192(1)$ $6953(1)$ $18662(1)$ $44(1)$ F (3) $11903(1)$ $6392(1)$ $17860(1)$ $42(1)$ F (4) $12666(1)$ $6624(1)$ $17745(1)$ $35(1)$ F (5) $11668(1)$ $7145(1)$ $17720(1)$ $35(1)$ F (6) $12134(1)$ $6814(1)$ $16806(1)$ $27(1)$ P (1) $10844(1)$ $5822(1)$ $11999(1)$ $16(1)$ P (2) $12166(1)$ $6888(1)$ $17735(1)$ $23(1)$ Ru (1) $10481(1)$ $6521(1)$ $14323(2)$ $35(1)$ O (2) $10000$ $5000$ $10634(2)$ $25(1)$	N(1)	10084(1)	7125(1)	11268(1)	17(1)
N (3)10651 (1)6336 (1)10488 (1)14 (1)N (4)11067 (1)6868 (1)11499 (1)16 (1)N (5)10530 (1)6830 (1)12716 (1)18 (1)O (1)10594 (1)5376 (1)11741 (1)23 (1)F (1)12430 (1)7375 (1)17605 (1)28 (1)F (2)12192 (1)6953 (1)18662 (1)44 (1)F (3)11903 (1)6392 (1)17860 (1)42 (1)F (4)12666 (1)6624 (1)17745 (1)35 (1)F (5)11668 (1)7145 (1)17720 (1)35 (1)F (6)12134 (1)6814 (1)16806 (1)27 (1)P (1)10844 (1)5822 (1)11999 (1)16 (1)P (2)12166 (1)6888 (1)17735 (1)23 (1)Ru (1)10481 (1)6521 (1)14323 (2)35 (1)O (2)10000500010634 (2)25 (1)	N(2)	9779(1)	6281(1)	11704(1)	14(1)
N (4)11067(1)6868(1)11499(1)16(1)N (5)10530(1)6830(1)12716(1)18(1)O (1)10594(1)5376(1)11741(1)23(1)F (1)12430(1)7375(1)17605(1)28(1)F (2)12192(1)6953(1)18662(1)44(1)F (3)11903(1)6392(1)17860(1)42(1)F (4)12666(1)6624(1)17745(1)35(1)F (5)11668(1)7145(1)17720(1)35(1)F (6)12134(1)6814(1)16806(1)27(1)P (1)10844(1)5822(1)11999(1)16(1)P (2)12166(1)6888(1)17735(1)23(1)Ru (1)10481(1)6521(1)14323(2)35(1)O (2)10000500010634(2)25(1)	N(3)	10651(1)	6336(1)	10488(1)	14(1)
N (5) $10530(1)$ $6830(1)$ $12718(1)$ $18(1)$ O(1) $10594(1)$ $5376(1)$ $11741(1)$ $23(1)$ F(1) $12430(1)$ $7375(1)$ $17605(1)$ $28(1)$ F(2) $12192(1)$ $6953(1)$ $18662(1)$ $44(1)$ F(3) $11903(1)$ $6392(1)$ $17860(1)$ $42(1)$ F(4) $12666(1)$ $6624(1)$ $17745(1)$ $35(1)$ F(5) $11668(1)$ $7145(1)$ $17720(1)$ $35(1)$ F(6) $12134(1)$ $6814(1)$ $16806(1)$ $27(1)$ P(1) $10844(1)$ $5822(1)$ $11999(1)$ $16(1)$ P(2) $12166(1)$ $6888(1)$ $17735(1)$ $23(1)$ Ru(1) $10481(1)$ $6521(1)$ $14323(2)$ $35(1)$ O(2) $10000$ $5000$ $10634(2)$ $25(1)$	N(4)	1106/(1) 10520(1)	6868(1) 6820(1)	11499(1)	16(1)
O(1)10394(1)3376(1)11741(1)23(1)F(1)12430(1)7375(1)17605(1)28(1)F(2)12192(1)6953(1)18662(1)44(1)F(3)11903(1)6392(1)17860(1)42(1)F(4)12666(1)6624(1)17745(1)35(1)F(5)11668(1)7145(1)17720(1)35(1)F(6)12134(1)6814(1)16806(1)27(1)P(1)10844(1)5822(1)11999(1)16(1)P(2)12166(1)6888(1)17735(1)23(1)Ru(1)10481(1)6521(1)11625(1)14(1)C(28)11224(1)6008(1)14323(2)35(1)O(2)10000500010634(2)25(1)	N(5)	10530(1) 10504(1)	6830(1) 5276(1)	12/10(1) 11741(1)	$\perp \delta (\perp)$
F(1) $12430(1)$ $7373(1)$ $17003(1)$ $220(1)$ $F(2)$ $12192(1)$ $6953(1)$ $18662(1)$ $44(1)$ $F(3)$ $11903(1)$ $6392(1)$ $17860(1)$ $42(1)$ $F(4)$ $12666(1)$ $6624(1)$ $17745(1)$ $35(1)$ $F(5)$ $11668(1)$ $7145(1)$ $17720(1)$ $35(1)$ $F(6)$ $12134(1)$ $6814(1)$ $16806(1)$ $27(1)$ $P(1)$ $10844(1)$ $5822(1)$ $11999(1)$ $16(1)$ $P(2)$ $12166(1)$ $6888(1)$ $17735(1)$ $23(1)$ $Ru(1)$ $10481(1)$ $6521(1)$ $11625(1)$ $14(1)$ $C(28)$ $11224(1)$ $6008(1)$ $14323(2)$ $35(1)$ $O(2)$ $10000$ $5000$ $10634(2)$ $25(1)$	$\cup$ (1) $\mathbb{F}$ (1)	10394(1) 12430(1)	7375(1)	11741(1) 17605(1)	23(1)
F(2) $12192(1)$ $00000(1)$ $100002(1)$ $141(1)$ $F(3)$ $11903(1)$ $6392(1)$ $17860(1)$ $42(1)$ $F(4)$ $12666(1)$ $6624(1)$ $17745(1)$ $35(1)$ $F(5)$ $11668(1)$ $7145(1)$ $17720(1)$ $35(1)$ $F(6)$ $12134(1)$ $6814(1)$ $16806(1)$ $27(1)$ $P(1)$ $10844(1)$ $5822(1)$ $11999(1)$ $16(1)$ $P(2)$ $12166(1)$ $6888(1)$ $17735(1)$ $23(1)$ $Ru(1)$ $10481(1)$ $6521(1)$ $11625(1)$ $14(1)$ $C(28)$ $11224(1)$ $6008(1)$ $14323(2)$ $35(1)$ $O(2)$ $10000$ $5000$ $10634(2)$ $25(1)$	F(2)	12430(1)	6953(1)	18662(1)	20(1)
F(4)12666(1)6624(1)17745(1)35(1)F(5)11668(1)7145(1)17720(1)35(1)F(6)12134(1)6814(1)16806(1)27(1)P(1)10844(1)5822(1)11999(1)16(1)P(2)12166(1)6888(1)17735(1)23(1)Ru(1)10481(1)6521(1)11625(1)14(1)C(28)11224(1)6008(1)14323(2)35(1)O(2)10000500010634(2)25(1)	F(3)	12192(1) 11903(1)	6392(1)	17860(1)	42(1)
F(5)11668(1)7145(1)17720(1)35(1)F(6)12134(1)6814(1)16806(1)27(1)P(1)10844(1)5822(1)11999(1)16(1)P(2)12166(1)6888(1)17735(1)23(1)Ru(1)10481(1)6521(1)11625(1)14(1)C(28)11224(1)6008(1)14323(2)35(1)O(2)10000500010634(2)25(1)	F(4)	12666(1)	6624(1)	17745(1)	35(1)
F(6)12134(1)6814(1)16806(1)27(1)P(1)10844(1)5822(1)11999(1)16(1)P(2)12166(1)6888(1)17735(1)23(1)Ru (1)10481(1)6521(1)11625(1)14(1)C (28)11224(1)6008(1)14323(2)35(1)O (2)10000500010634(2)25(1)	F(5)	11668(1)	7145(1)	17720(1)	35(1)
P(1)10844(1)5822(1)11999(1)16(1)P(2)12166(1)6888(1)17735(1)23(1)Ru(1)10481(1)6521(1)11625(1)14(1)C(28)11224(1)6008(1)14323(2)35(1)O(2)10000500010634(2)25(1)	F(6)	12134(1)	6814(1)	16806(1)	27(1)
P(2)12166(1)6888(1)17735(1)23(1)Ru(1)10481(1)6521(1)11625(1)14(1)C(28)11224(1)6008(1)14323(2)35(1)O(2)10000500010634(2)25(1)	P(1)	10844(1)	5822(1)	11999(1)	16(1)
Ru (1)10481 (1)6521 (1)11625 (1)14 (1)C (28)11224 (1)6008 (1)14323 (2)35 (1)O (2)10000500010634 (2)25 (1)	P(2)	12166(1)	6888(1)	17735(1)	23(1)
C (28)11224 (1)6008 (1)14323 (2)35 (1)O (2)10000500010634 (2)25 (1)	Ru(1)	10481(1)	6521(1)	11625(1)	14(1)
O(2) 10000 5000 10634(2) 25(1)	C(28)	11224(1)	6008(1)	14323(2)	35(1)
	0(2)	10000	5000	10634(2)	25(1)

C(1)-N(1)	1.349(4)
$\alpha(1) = \alpha(2)$	1 27(1)
C(1) = C(2)	1.3/6(4)
C(1) - H(1)	0 9500
0 (2) = (2)	1.000(4)
C(3) - C(2)	1.3/8(4)
C(3) = C(4)	1 380(4)
C(3) = C(4)	1.300(4)
C(3)-H(3)	0.9500
C(2) $T(2)$	0 0500
C(Z) = H(Z)	0.9500
C(4) - C(5)	1.397(4)
O(A) = U(A)	
C(4) - H(4)	0.9500
C(5) - N(1)	1 348(4)
	1.010(1)
C(5)-C(6)	1.4/1(4)
C(6) = N(2)	1 380(3)
C(0) $N(2)$	1.300(3)
C(6)-C(7)	1.382(4)
C(7) = C(8)	1 382(1)
C(7) $C(0)$	1.302(4)
С(7)-Н(7)	0.9500
C(0) = C(0)	1 201 (1)
C(0) = C(9)	1.301(4)
C(8)-H(8)	0.9500
$\alpha(0) = \alpha(10)$	1 202(4)
C(9) = C(10)	1.383(4)
C(9)-H(9)	0.9500
$\alpha(10) \rightarrow 100$	1 242 (2)
C(10) - N(2)	1.343(3)
C(10) - H(10)	0.9500
C(11)-N(3)	1.341(4)
C(11) - C(12)	1 383(4)
	1.303(4)
C(11)-H(11)	0.9500
C(12) - C(13)	1 383(4)
C(12) $C(13)$	1.303(4)
C(12)-H(12)	0.9500
C(13) = C(14)	1 386(4)
C(13) = C(14)	1.300(4)
С(13)-Н(13)	0.9500
C(14) = C(15)	1 296(4)
C(14) = C(15)	1.300(4)
C(14)-H(14)	0.9500
$\alpha(1 \Gamma) \rightarrow \alpha(2)$	1 270 ( 4 )
C(15) - N(3)	1.3/9(4)
C(15) - C(16)	1,475(4)
O(10) O(10)	
C(16) - N(4)	1.355(4)
C(16) - C(17)	1,388(4)
c(10) c(1)	
C(1/) - C(18)	1.38/(4)
C(17) - H(17)	0 9500
O(1,) $H(1,)$	
C(18)-C(19)	1.384(4)
C(18) - H(18)	0 9500
0(10) n(10)	
C(19)-C(20)	1.391(4)
C(19) - H(19)	0 9500
	0.9900
C(20)-N(4)	1.362(4)
C(20) - C(21)	1 459(4)
C(20) C(21)	1.455(4)
C(21)-N(5)	1.370(4)
C(21) - C(22)	1 384(4)
C(ZI) = C(ZZ)	1.304(4)
C(22)-C(23)	1.368(5)
C(22) = H(22)	0 9500
C(ZZ) = H(ZZ)	0.9300
C(23)-C(24)	1.369(4)
C(23) _U(22)	0 0500
$C(23) = \pi(23)$	0.9300
C(24)-C(25)	1.378(4)
(24) $(24)$	
$\cup (24) = H(24)$	0.9500
C(25)-N(5)	1.348(4)
U(23) = H(23)	0.9500
C(26)-C(31)	1.392(4)
C(26) - C(27)	1.394(4)
C(26) - P(1)	1.838(3)
a ( ) ] ) a ( ) ) )	1 202/51
C(27)-C(28)	1.383(5)

## Table 7. Bond lengths [A] and angles [deg] for complex 3.

C (29) - C (30) $C (29) - C (28)$ $C (29) - H (29)$ $C (30) - C (31)$ $C (30) - H (30)$ $C (31) - H (31)$ $C (32) - C (37)$ $C (32) - C (37)$ $C (32) - C (33)$ $C (32) - P (1)$ $C (33) - C (34)$ $C (33) - H (33)$ $C (34) - C (35)$ $C (34) - C (35)$ $C (34) - H (34)$ $C (35) - C (36)$ $C (35) - H (35)$ $C (36) - C (37)$ $C (36) - H (36)$ $C (37) - H (37)$ $N (1) - Ru (1)$ $N (2) - Ru (1)$ $N (2) - Ru (1)$ $N (3) - Ru (1)$ $N (4) - Ru (1)$ $N (4) - Ru (1)$ $N (5) - Ru (1)$ $O (1) - P (1)$ $F (1) - P (2)$ $F (2) - P (2)$ $F (3) - P (2)$ $F (4) - P (2)$ $F (5) - P (2)$ $F (6) - P (2)$ $P (1) - Ru (1)$ $C (28) - H (28)$ $O (2) - H (2B)$	$\begin{array}{c} 1.373(5)\\ 1.377(5)\\ 0.9500\\ 1.388(5)\\ 0.9500\\ 0.9500\\ 1.391(4)\\ 1.401(4)\\ 1.401(4)\\ 1.843(3)\\ 1.376(4)\\ 0.9500\\ 1.366(5)\\ 0.9500\\ 1.366(5)\\ 0.9500\\ 1.384(5)\\ 0.9500\\ 1.394(5)\\ 0.9500\\ 2.142(2)\\ 2.112(2)\\ 2.067(2)\\ 1.949(2)\\ 2.063(2)\\ 1.5199(19)\\ 1.5918(18)\\ 1.5928(19)\\ 1.6084(19)\\ 1.6084(19)\\ 1.6020(17)\\ 2.3260(8)\\ 0.9500\\ 0.79(3)\\ \end{array}$
N(1) - C(1) - C(2) $N(1) - C(1) - H(1)$ $C(2) - C(1) - H(1)$ $C(2) - C(3) - C(4)$ $C(2) - C(3) - C(4)$ $C(2) - C(3) - H(3)$ $C(1) - C(2) - C(3)$ $C(1) - C(2) - H(2)$ $C(3) - C(2) - H(2)$ $C(3) - C(4) - C(5)$ $C(3) - C(4) - H(4)$ $C(5) - C(4) - H(4)$ $C(5) - C(4) - H(4)$ $N(1) - C(5) - C(6)$ $C(4) - C(5) - C(6)$ $N(2) - C(6) - C(7)$ $N(2) - C(6) - C(7)$ $N(2) - C(6) - C(5)$ $C(7) - C(6) - C(5)$ $C(6) - C(7) - H(7)$ $C(8) - C(7) - H(7)$ $C(9) - C(8) - H(8)$ $C(7) - C(8) - H(8)$ $C(7) - C(9) - H(9)$ $C(10) - C(9) - H(9)$	122.8(3) $118.6$ $118.6$ $119.6(3)$ $120.2$ $120.2$ $120.7$ $120.7$ $120.7$ $120.4$ $120.4$ $121.2(3)$ $115.5(2)$ $123.3(3)$ $121.3(2)$ $125.5(2)$ $123.1(2)$ $120.3(3)$ $119.9$ $119.9$ $119.9$ $119.9$ $119.9$ $119.9$ $119.0(3)$ $120.5$ $120.5$

N(2) - C(10) - C(9)	123.6(3)
N(2) - C(10) - H(10)	118 2
C(9) - C(10) - H(10)	118 2
N(3) = C(11) = C(12)	123 0(3)
N(3) = C(11) = U(11)	118 5
R(3) = C(11) = II(11)	110.J
C(12) - C(11) - H(11)	110.0
C(13) = C(12) = C(11)	118.9(3)
C(13) - C(12) - H(12)	120.6
C(11) - C(12) - H(12)	120.6
C(12) - C(13) - C(14)	119.3(3)
С(12)-С(13)-Н(13)	120.4
С(14) – С(13) – Н(13)	120.4
C(13) - C(14) - C(15)	119.6(3)
C(13) - C(14) - H(14)	120.2
C(15) - C(14) - H(14)	120.2
N(3) - C(15) - C(14)	121.1(3)
N(3) - C(15) - C(16)	114.9(2)
C(14) - C(15) - C(16)	123.9(3)
N(4)-C(16)-C(17)	120.1(3)
N(4)-C(16)-C(15)	112.7(2)
C(17)-C(16)-C(15)	127.2(3)
C(18)-C(17)-C(16)	118.8(3)
С(18)-С(17)-Н(17)	120.6
С(16)-С(17)-Н(17)	120.6
C(19)-C(18)-C(17)	120.4(3)
С(19)-С(18)-Н(18)	119.8
С(17)-С(18)-Н(18)	119.8
C(18)-C(19)-C(20)	119.7(3)
С(18)-С(19)-Н(19)	120.2
С(20)-С(19)-Н(19)	120.2
N(4)-C(20)-C(19)	118.9(3)
N(4)-C(20)-C(21)	113.5(2)
C(19)-C(20)-C(21)	127.5(3)
N(5)-C(21)-C(22)	120.5(3)
N(5)-C(21)-C(20)	114.9(2)
C(22)-C(21)-C(20)	124.6(3)
C(23)-C(22)-C(21)	120.1(3)
С(23)-С(22)-Н(22)	120.0
С(21)-С(22)-Н(22)	120.0
C(22)-C(23)-C(24)	119.4(3)
С(22)-С(23)-Н(23)	120.3
С(24)-С(23)-Н(23)	120.3
C(23)-C(24)-C(25)	119.3(3)
С(23)-С(24)-Н(24)	120.3
С(25)-С(24)-Н(24)	120.3
N(5)-C(25)-C(24)	122.1(3)
N(5)-C(25)-H(25)	118.9
С(24)-С(25)-Н(25)	118.9
C(31)-C(26)-C(27)	118.2(3)
C(31)-C(26)-P(1)	117.0(2)
C(27)-C(26)-P(1)	124.7(2)
C(28)-C(27)-C(26)	120.5(3)
С(28)-С(27)-Н(27)	119.7
С(26)-С(27)-Н(27)	119.7
C(30)-C(29)-C(28)	120.0(3)
С(30)-С(29)-Н(29)	120.0
С(28)-С(29)-Н(29)	120.0
C(29)-C(30)-C(31)	119.9(3)
С(29)-С(30)-Н(30)	120.0
С(31)-С(30)-Н(30)	120.0
C(30)-C(31)-C(26)	120.9(3)

C(30) = C(31) = U(31)	119 6
C(30) = C(31) = II(31)	119.0
C(26)-C(31)-H(31)	119.6
C(37) - C(32) - C(33)	118.1(3)
C(37) - C(32) - P(1)	$\perp \perp / . \angle ( \angle )$
C(33) - C(32) - P(1)	124.7(2)
C(34) = C(33) = C(32)	121 0 (3)
0 (34) -0 (33) -0 (32)	121.0(3)
С (34) – С (33) – Н (33)	119.5
С(32)-С(33)-Н(33)	119.5
C(25) = C(24) = C(22)	120 0(2)
C(33) = C(34) = C(33)	120.0(3)
C(35)-C(34)-H(34)	119.6
С(33)-С(34)-Н(34)	119.6
C(34) - C(35) - C(36)	110 3 (3)
C(34) = C(33) = C(30)	119.3(3)
C(34)-C(35)-H(35)	120.4
С(36)-С(35)-Н(35)	120.4
C(35) = C(36) = C(37)	120 8 (3)
C(33) = C(30) = C(37)	120.0(3)
С(35)-С(36)-Н(36)	119.6
С(37)-С(36)-Н(36)	119.6
C(32) = C(37) = C(36)	120 0(3)
C(32) = C(37) = C(30)	120.0(3)
C(32) - C(37) - H(37)	120.0
С(36)-С(37)-Н(37)	120.0
C(5) = N(1) = C(1)	118 7(2)
	110.7(2)
C(5) - N(1) - Ru(1)	115.00(18)
C(1)-N(1)-Ru(1)	125.5(2)
C(10) = N(2) = C(6)	117 2(2)
C(10) N(2) C(0)	
C(10) - N(2) - Ru(1)	127.54(18)
C(6)-N(2)-Ru(1)	115.26(17)
C(11) = N(3) = C(15)	118 2 (2)
C(11) = N(3) = C(13)	110.2(2)
C(11) – N(3) – Ru(1)	128.77(19)
C(15)-N(3)-Ru(1)	113.05(18)
C(16) = N(4) = C(20)	122 1 (2)
C(10) N(4) C(20)	110 00 (10)
C(16) - N(4) - Ru(1)	119.27(19)
C(20)-N(4)-Ru(1)	118.08(19)
C(25) = N(5) = C(21)	1185(2)
C(25) N(5) C(21)	100.0(2)
C(25) - N(5) - Ru(1)	128.28(19)
C(21)-N(5)-Ru(1)	113.24(19)
O(1) - P(1) - C(26)	105 78(13)
O(1) P(1) O(20)	105.70(19)
O(1) - P(1) - C(32)	105.45(12)
C(26) - P(1) - C(32)	103.22(14)
$O(1) - P(1) - R_{11}(1)$	115 26(8)
O(2) = D(1) = D(1)	112 (1 (0)
C(26) = P(1) = Ru(1)	113.61(9)
C(32)-P(1)-Ru(1)	112.45(9)
F(1) - P(2) - F(2)	90.86(10)
$\nabla (1) - \nabla (2) - \nabla (5)$	00 09 (10)
F(1) - F(2) - F(3)	90.98(10)
F(2) - P(2) - F(5)	90.21(10)
F(1) - P(2) - F(6)	90.18(9)
E(2) = D(2) = E(6)	170 05(12)
F(2) - F(2) - F(0)	178.95(12)
F(5) - P(2) - F(6)	89.63(10)
F(1) - P(2) - F(4)	89.48(10)
= (-) = (-) = (-) = (-) = (-)	00 19(10)
F(2) - F(2) - F(4)	90.18(10)
F(5) - P(2) - F(4)	179.39(11)
F(6)-P(2)-F(4)	89.98(10)
F(1) - P(2) - F(3)	179 25(12)
r(r) = r(r)	
F(2)-P(2)-F(3)	89.55(11)
F(5)-P(2)-F(3)	89.51(10)
F(6) - P(2) - F(3)	29 /1 /1 O
-107 $-107$ $-107$	
F'(4) - F(2) - F'(3)	90.02(10)
N(4)-Ru(1)-N(5)	79.95(10)
$N(4) - R_{11}(1) - N(3)$	79 22(9)
$\mathbf{T}(\mathbf{T}) = \mathbf{T}(\mathbf{T}) \mathbf{T}(\mathbf{T})$	150 04 (0)
N ( ) – KU ( 1 ) – N ( 3 )	159.84(9)
N(4)-Ru(1)-N(2)	167.95(8)
$N(5) - R_{11}(1) - N(2)$	98 27 (9)

Table 8. Anisotropic displacement parameters  $(A^2 \times 10^3)$  for complex 3.

The anisotropic displacement factor exponent takes the form: -2 pi^2 [ h^2 a\*^2 U11 + ... + 2 h k a\* b\* U12 ]

	U11	U22	U33	U23	U13	U12
C (1)	21(2)	21(2)	25(2)	-3(2)	-4(1)	-3(2)
C(3)	31(2)	18(2)	42(2)	-4(2)	-13(2)	7(2)
C(2)	30(2)	18(2)	42(2)	4(2)	-13(2)	0(2)
C(4)	20(2)	27(2)	27(2)	-7(2)	-6(1)	-1(2)
C(5)	19(2)	21(2)	12(2)	-4(1)	-2(1)	5(1)
C(6)	18(2)	21(2)	10(2)	-5(2)	1(2)	1(1)
C(7)	13(2)	25(2)	21(2)	-6(2)	-6(2)	5(1)
C(8)	13(2)	34(2)	18(2)	-3(2)	0(2)	0(1)
C(9)	20(2)	23(2)	13(2)	-3(1)	4(1)	-6(1)
C(10)	18(2)	21(2)	13(2)	-5(1)	0(1)	2(1)
C(11)	15(2)	17(2)	21(2)	4(2)	-3(1)	0(1)
C(12)	21(2)	22(2)	15(2)	-3(1)	-5(2)	4(1)
C(13)	30(2)	23(2)	11(2)	-2(1)	-1(1)	6(2)
C(14)	18(2)	20(2)	23(2)	5(1)	6(2)	5(1)
C(15)	12(2)	15(2)	21(2)	1(1)	1(1)	4(1)
C(16)	17(2)	19(2)	19(2)	4(1)	1(1)	1(1)
C(17)	23(2)	27(2)	24(2)	-1(2)	4(2)	-3(2)
C(18)	19(2)	28(2)	39(2)	-3(2)	2(2)	-7(2)
C(19)	20(2)	22(2)	36(2)	-9(2)	-5(2)	-4(2)
C(20)	15(2)	19(2)	24(2)	-2(2)	-5(1)	3(1)
C(21)	19(2)	19(2)	21(2)	-6(1)	-10(2)	1(1)
C(22)	30(2)	25(2)	28(2)	-7(2)	-5(2)	-4(2)
C(23)	41(2)	41(2)	19(2)	-10(2)	-5(2)	0(2)
C(24)	35(2)	38(2)	20(2)	-2(2)	4(2)	0(2)
C(25)	25(2)	25(2)	18(2)	-5(2)	-1(2)	0(1)
C(26)	19(2)	21(2)	16(2)	2(2)	4(1)	7(1)
C(27)	28(2)	29(2)	21(2)	5(2)	-4(2)	1(2)
C(29)	71(3)	42(2)	15(2)	4(2)	4(2)	16(2)
C(30)	63(2)	32(2)	27(2)	10(2)	24(2)	4(2)
C(31)	32(2)	30(2)	29(2)	1(2)	11(2)	3(2)
C(32)	23(2)	19(2)	13(2)	2(2)	1(2)	9(1)
C(33)	17(2)	27(2)	24(2)	2(1)	-2(1)	6(1)

C(34)	23(2)	41(2)	29(2)	12(2)	-2(2)	2(2)
C(35)	28(2)	44(2)	47(2)	10(2)	17(2)	8(2)
C(36)	56(3)	37(2)	33(2)	-3(2)	21(2)	16(2)
C(37)	38(2)	23(2)	23(2)	3(2)	6(2)	3(2)
N(1)	18(2)	16(2)	16(1)	-2(1)	-1(1)	-1(1)
N(2)	20(1)	14(1)	8(1)	-2(1)	-1(1)	1(1)
N(3)	15(1)	14(1)	14(1)	-1(1)	-3(1)	3(1)
N(4)	12(1)	18(1)	17(2)	-1(1)	-5(1)	1(1)
N(5)	19(1)	21(2)	14(1)	-1(1)	-4(1)	3(1)
0(1)	22(1)	17(1)	29(1)	-3(1)	-8(1)	-1(1)
F(1)	31(1)	20(1)	33(1)	-1(1)	4(1)	-3(1)
F(2)	37(1)	74(2)	19(1)	0(1)	-1(1)	-22(1)
F(3)	42(1)	35(1)	48(1)	14(1)	-15(1)	-21(1)
F(4)	26(1)	28(1)	50(1)	2(1)	-8(1)	4(1)
F(5)	23(1)	50(1)	33(1)	-13(1)	4(1)	5(1)
F(6)	31(1)	31(1)	20(1)	-7(1)	2(1)	6(1)
P(1)	15(1)	19(1)	15(1)	0(1)	-2(1)	1(1)
P(2)	22(1)	26(1)	22(1)	1(1)	0(1)	-4(1)
Ru(1)	13(1)	16(1)	13(1)	-1(1)	-2(1)	0(1)
C(28)	47(2)	35(2)	23(2)	-4(2)	-9(2)	9(2)
0(2)	23(2)	36(2)	15(2)	0	0	-5(2)



Figure S7 : <sup>31</sup>P NMR spectra of complex **3** in CD<sub>3</sub>CN at 298K.



Figure S8 : <sup>1</sup>H NMR spectra of complex **3** in  $CD_2Cl_2$  at 298K.



Figure S9 : <sup>1</sup>H NMR spectra of complex **3** in  $CD_2Cl_2$  at 183K.



Figure S10 :  ${}^{1}H{}^{31}P{}$  (top) and  ${}^{1}H$  NMR (under) spectra of complex 3 in CD<sub>2</sub>Cl<sub>2</sub> at 183K.

Luminescence quantum yields have been calculated using the optically dilute method,<sup>6</sup> employing  $[Ru(bpy)_3]^{2+}$  in air-equilibrated aqueous solution as quantum yield standard (0.028).<sup>7</sup> Experimental uncertainties on the absorption and photophysical data are as follows: absorption maxima, 2 nm; molar absorption, 20%; luminescence maxima, 4 nm; luminescence lifetimes, 10%; luminescence quantum yields, 20%.



Figure S11. Luminescence spectra of **1** in acetonitrile at room temperature (solid line) and in butyronitrile at 77 K (dashed line). Spectra are normalized and uncorrected for PMT response.

	298 K <sup>a</sup>			77 K <sup>b</sup>		
	Absorption <sup>c</sup> $\lambda$ , nm ( $\epsilon$ , M <sup>-1</sup> cm <sup>-1</sup> )	Emission <sup>d</sup> λmax, nm	Em τ, ns	Ет ф(10^-4)	Emission <sup>d</sup> λmax, nm	Em τ (μs)
1	480 (5560)	705 (745)	55	8	658 (685)	3.6
2	436 (11950)	no detectable emission				
3	438 (11600)	no detectable emission				

Table 9. Selected photophysical data of phosphoryl complexes 1, 2 and 3.

(a) Data at 298 K are in acetonitrile; (b) Emission data at 77 K are in butyronitrile; (c) Only the lowest-energy maximum is reported; (d) Corrected values in parenthesis.

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