Supplementary data for

NOVEL CLASS OF FUNCIONALIZED IONIC LIQUIDS WITH GRAFTED CMPO-MOIETIES FOR ACTINIDES AND RARE-EARTH ELEMENTS RECOVERY.

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1.1. Experimental details

2-(Diphenylphosphinyl)-N-[3-(1*H*-imidazol-1-yl)propyl]-acetamide (3). A mixture of ethyl(diphenylphosphoryl)acetate (4.6 g, 0.016 mol) and 3-(1*H*-imidazol-1-yl)-1-propanamine (2.8 g, 0.023 mol) in 5 mL of anhydrous EtOH was heated in a sealed tube in a boiling water bath for 72 h. The tube was opened, the solvent was removed *in vacuo*, and the residue was recrystallized from EtOAc-EtOH (10:1) to give **3** as a white solid; yield: 4.7 g (81%); mp 145-146 °C (EtOAc-EtOH). IR (cm^{-1}): 1438 (ν_{CH2}), 1180 ($\nu_{P=O}$), 1661 ($\nu_{C=O}$), 3263, 1546 (ν_{NH}). ^{1}H NMR (400 MHz, $CDCl_3$, ppm, J/Hz): 1.83 (q, 2H, C$\underline{H}_2$CH$_2$NHC(O), $^3J_{H-H}$=6.6); 3.20 (appeared qv, 2H, C$\underline{H}_2$NHC(O), $^3J_{H-H}$=6.4); 3.31 (d, 2H, PCH$_2$, $^2J_{P-H}$=12.4); 3.69 (t, 2H, C$\underline{H}_2$CH$_2$CH$_2$NHC(O), $^3J_{H-H}$=7.1); 6.79 (br. s, 1H, C^{5}H in Im); 7.00 (br. s, 1H, C^{4}H in Im); 7.46 (br. s, 1H, NH); 7.47-7.53 (m, 4H, *m*-C$_6$H$_5$P); 7.54-7.60 (м, 2H, *p*-C$_6$H$_5$P); 7.70-7.78 (m, 4H, *o*-C$_6$H$_5$P); 7.32 (br. s, 1H, N=CH-N). ^{31}P NMR (162 MHz, $CDCl_3$, ppm): 30.41 ppm. ^{13}C NMR (75.47 MHz, $CDCl_3$): δ 30.32 (C$\underline{H}_2$CH$_2$N), 35.98 (NHCH$_2$), 38.41 (d, PCH$_2$, $^1J_{PC}$=60.9 Hz), 43.47 (N$_{Im}$-CH$_2$), 118.46 (C^4 (Im)), 128.38 (d, *m*-C in C$_6$H$_5$, $^3J_{PC}$= 12.1 Hz), 128.72 (C^5 (Im)), 130.29 (d, *o*-C in C$_6$H$_5$, $^2J_{PC}$=9.9 Hz), 131.16 (d, ipso-C in C$_6$H$_5$, $^1J_{PC}$=103.2 Hz), 131.97 (*p*-C in C$_6$H$_5$), 136.71 (C^2 (Im)), 164.59 (d, C(O), $^2J_{PC}$=4.9 Hz). Anal. Calcd for $C_{20}H_{22}N_3O_2P$: C, 65.39; H, 6.04; N, 11.44; P, 8.43. Found: C, 65.24; H, 5.86; N, 11.39; P, 8.13.

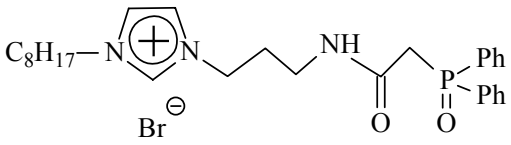
Table S1. Selected bond lengths and angles in crystals of **4d** and **6c**.

Lengths, Å	**4d**	**6c**	Angles, °	**4d**	**6c**
P(1)-O(1)	1.4907(17)	1.4944(14)	O(1)P(1)C(10)	112.34(11)	116.22(9)
N(1)-C(2)	1.326(3)	1.322(2)	N(1)C(2)N(3)	108.3(2)	109.19(18)
C(2)-N(3)	1.332(3)	1.325(2)	C(2)N(3)C(4)	108.9(2)	108.19(17)
N(3)-C(4)	1.371(3)	1.376(2)	N(3)C(4)C(5)	107.1(2)	106.99(18)
C(4)-C(5)	1.351(3)	1.349(3)	C(4)C(5)N(1)	106.9(2)	107.23(17)
C(5)-N(1)	1.378(3)	1.371(2)	C(5)N(1)C(2)	108.85(19)	108.40(17)
N(1)-C(6)	1.469(3)	1.473(2)	C(2)N(1)C(6)	125.5(2)	124.16(17)
C(6)-C(7)	1.521(4)	1.530(3)	N(1)C(6)C(7)	110.6(2)	110.96(16)
C(7)-C(8)	1.518(3)	1.522(3)	C(6)C(7)C(8)	114.0(2)	114.72(16)
N(4)-C(8)	1.453(3)	1.450(2)	C(7)C(8)N(4)	110.5(2)	112.04(16)
N(4)-C(9)	1.336(3)	1.346(2)	C(8)N(4)C(9)	123.5(2)	123.76(16)
C(9)-O(2)	1.230(3)	1.238(2)	O(2)C(9)N(4)	123.8(2)	123.65(18)

Table S2. Crystal data and structure refinement parameters for **4d** and **6c**.

Compound	**4d**	**6c**
Empirical formula	$C_{60}H_{86}Br_2Cl_6N_6O_5P_2$	$C_{26}H_{35}F_6N_3O_2P_2$
Formula weight	1405.81	597.51
Crystal colour, habit	colorless, prism	colorless, needle
Crystal size (mm)	0.18 × 0.20 × 0.25	0.08 × 0.10 × 0.45
Crystal system	Orthorhombic	Triclinic
Space group	Pbca	P-1
a (Å)	23.9357(16)	5.9341(9)
b (Å)	11.7625(8)	15.819(3)
c (Å)	25.1174(17)	16.393(3)
α (°)	–	65.857(3)
β (°)	–	88.250(4)
γ (°)	–	80.353(4)
V (Å^3)	7071.6(8)	1383.1(4)
$Z(Z')$	4(0.5)	2(1)
$F(000)$	2920	624
D_{calc} (g cm^{-1})	1.320	1.435
Linear absorption, μ (cm^{-1})	14.66	2.28
$2\theta_{max}$ (°)	58	54
Completeness of dataset (%)	99.9	98.0
Reflections measured	82400	8923
Independent reflections	9385 [R_{int} = 0.0622]	5935 [R_{int} = 0.0284]
Observed reflections [$I > 2\sigma(I)$]	6976	3936
Parameters	378	356
Final $R(F_{hkl})$: R_1	0.0385	0.0403
wR_2	0.1233	0.0677
GOF	1.007	1.004
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.808, −0.602	0.365, −0.391

Spectroscopy of compounds



4d

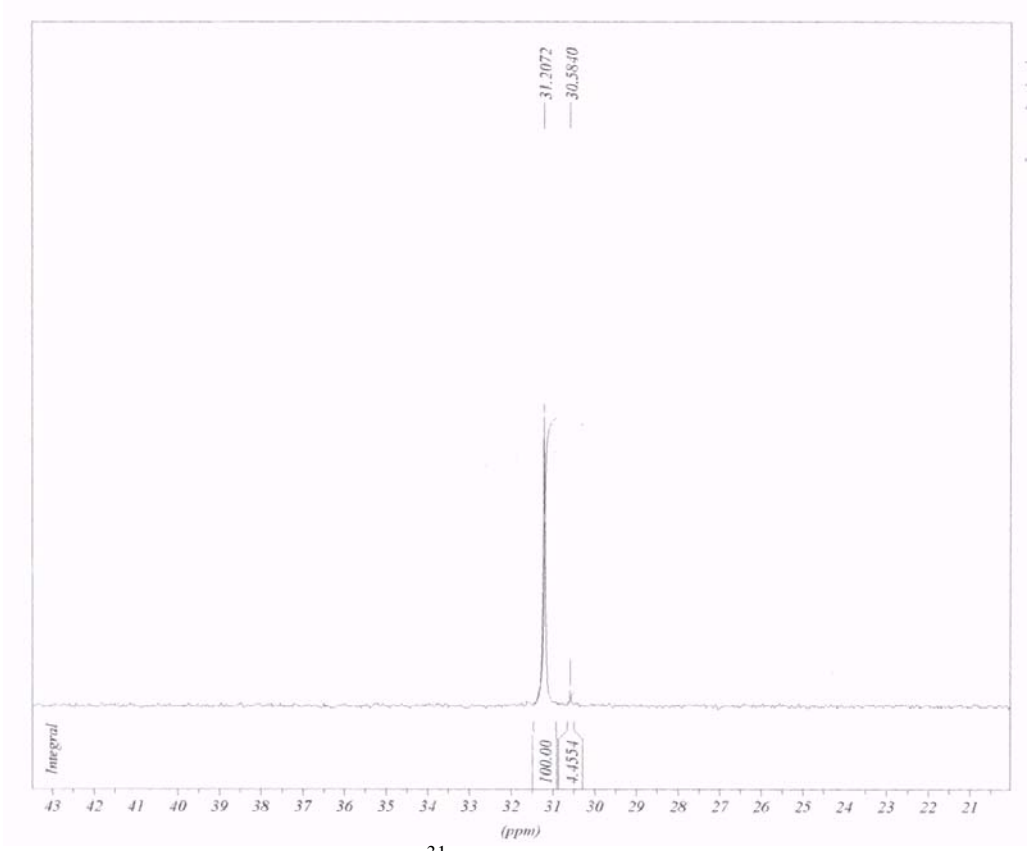
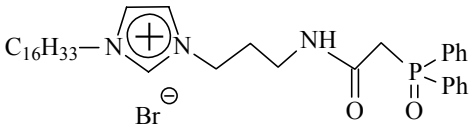


Fig S1. The ^{31}P spectrum for ligand **4d**



4f

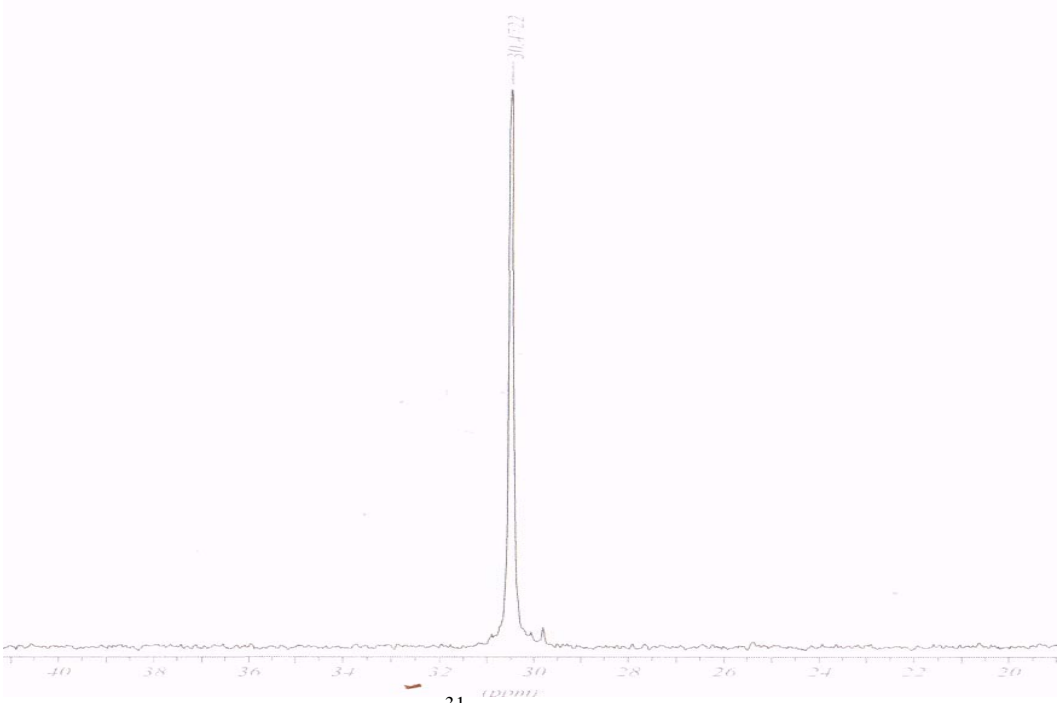
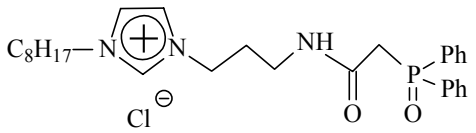


Fig S2. The ^{31}P spectrum for ligand **4f**



5d

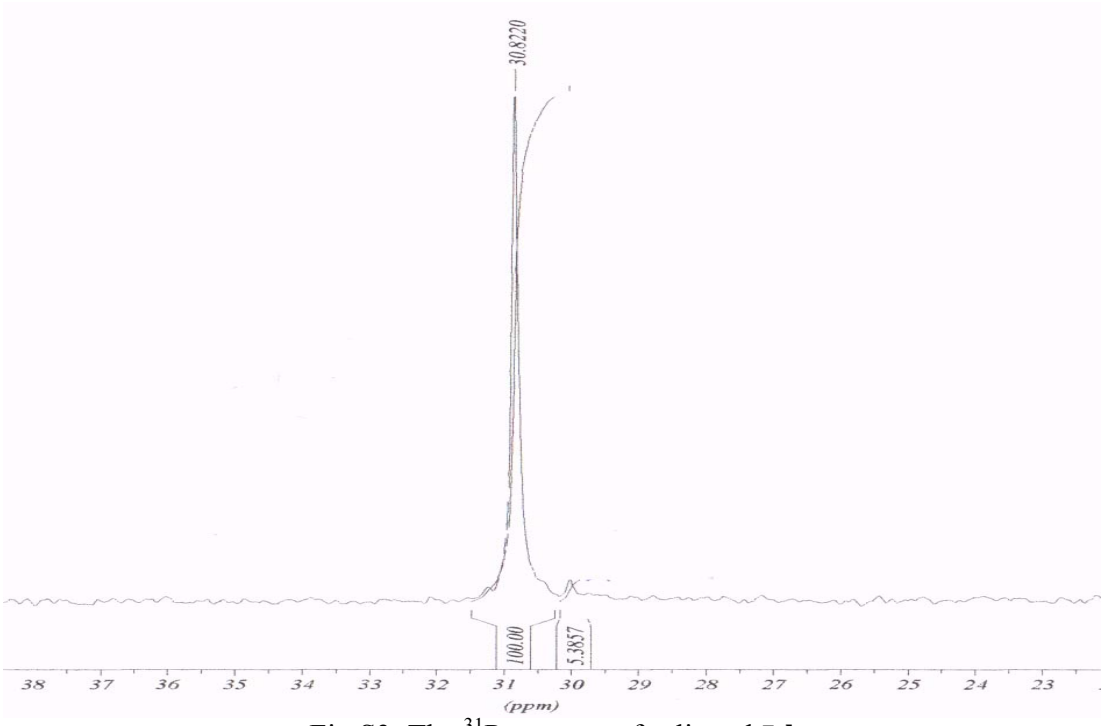
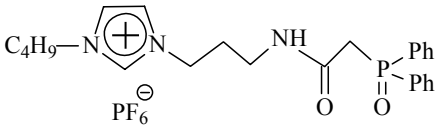


Fig S3. The ^{31}P spectrum for ligand **5d**



6b

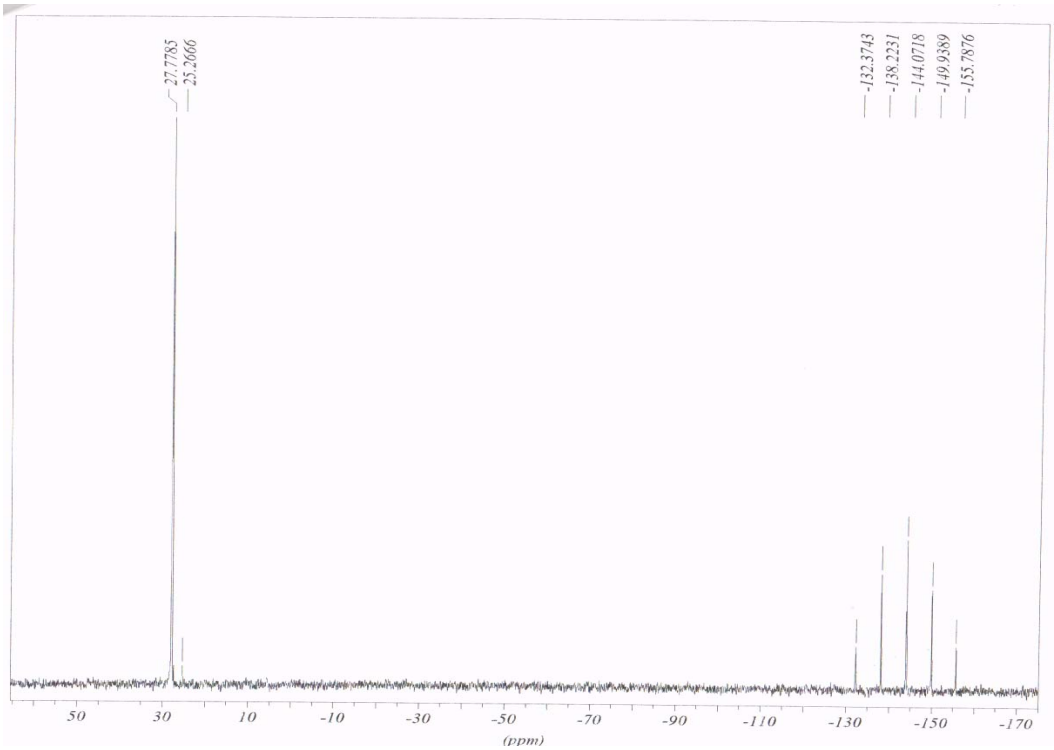


Fig S4. The ^{31}P spectrum for ligand **6b**

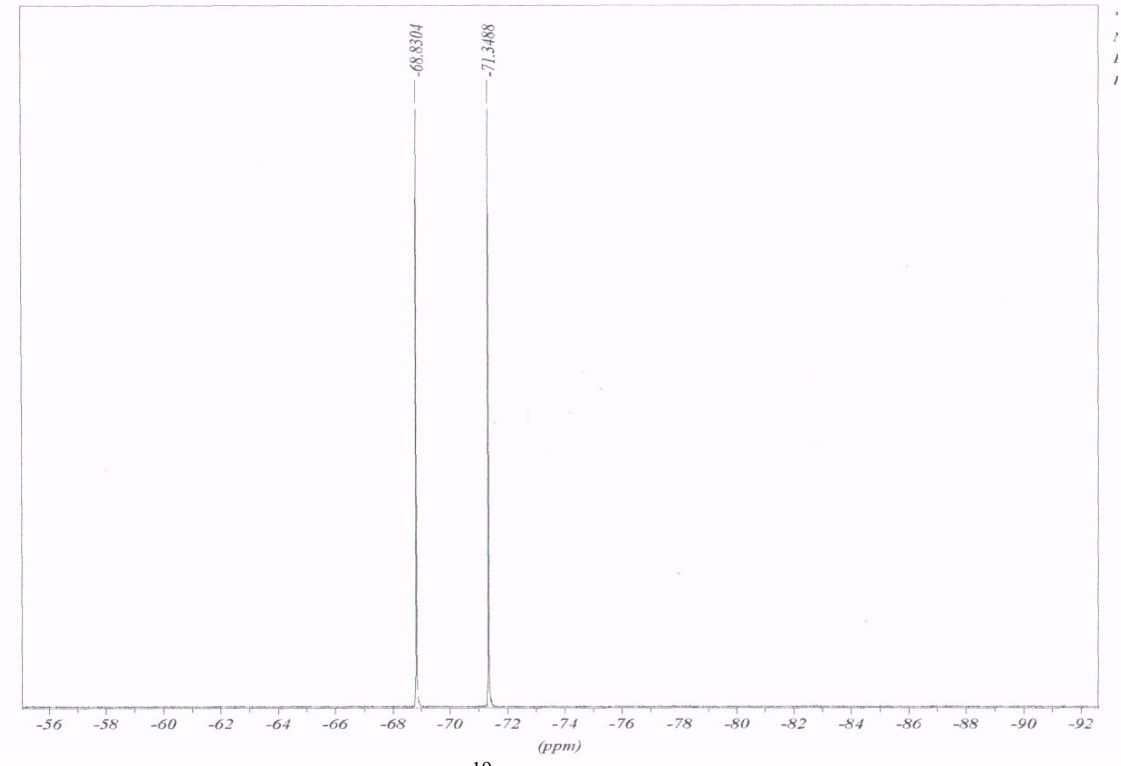
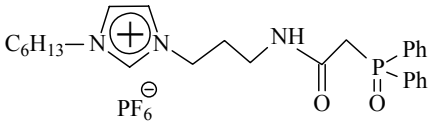


Fig S5. The ^{19}F spectrum for ligand **6b**



6c

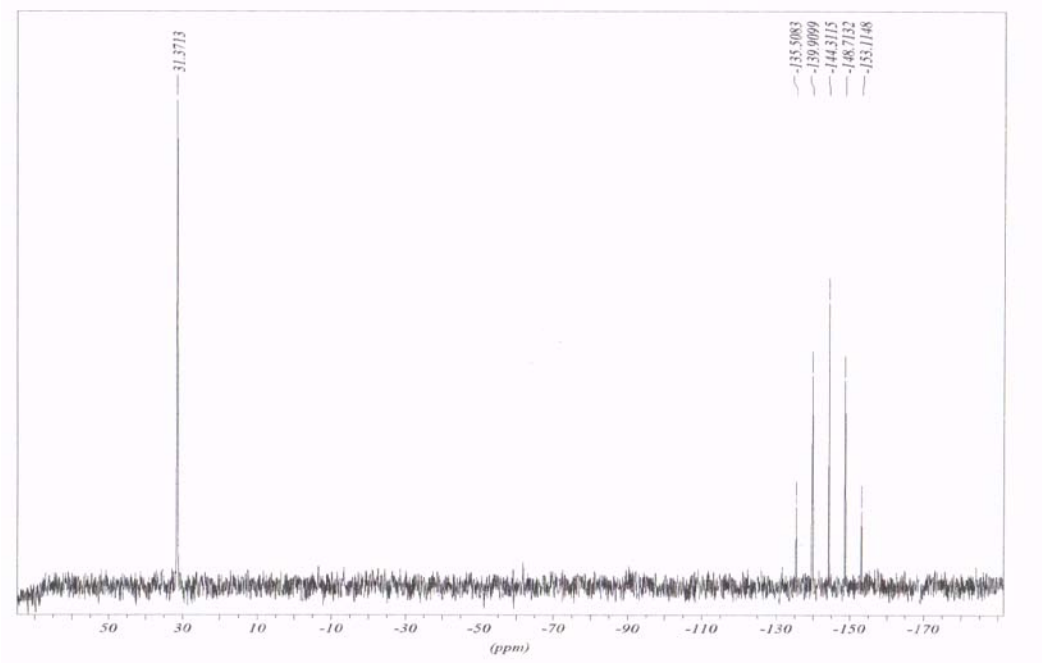


Fig S6. The ^{31}P spectrum for ligand **6c**

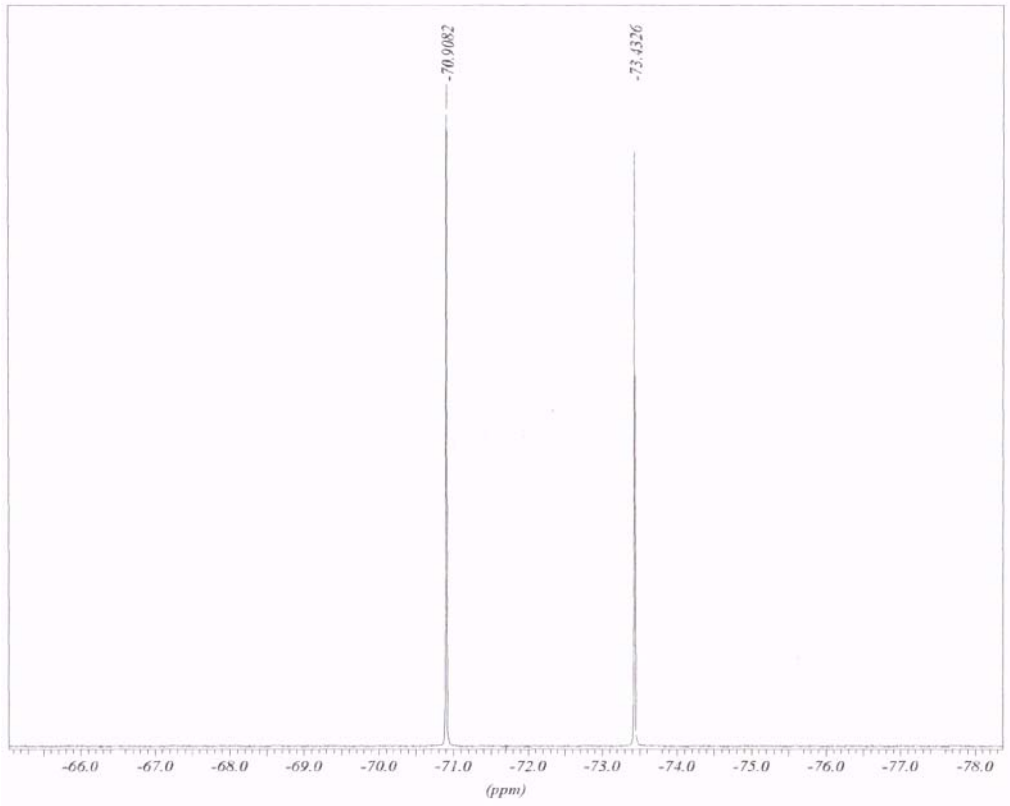
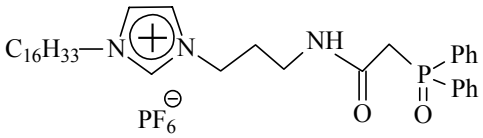


Fig S7. The ^{19}F spectrum for ligand **6c**



6f

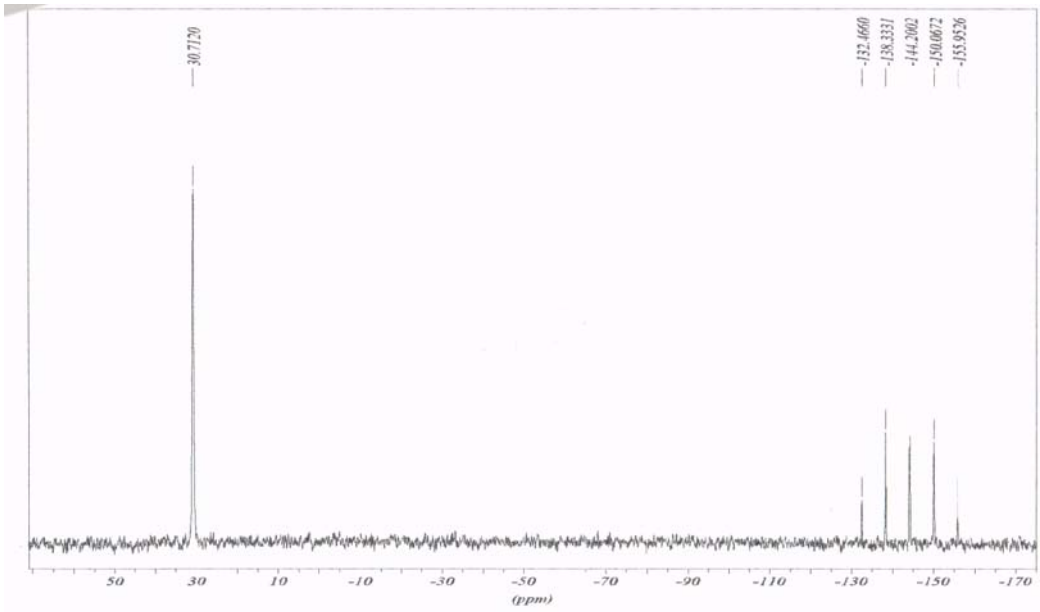


Fig S8. The ^{31}P spectrum for ligand **6f**

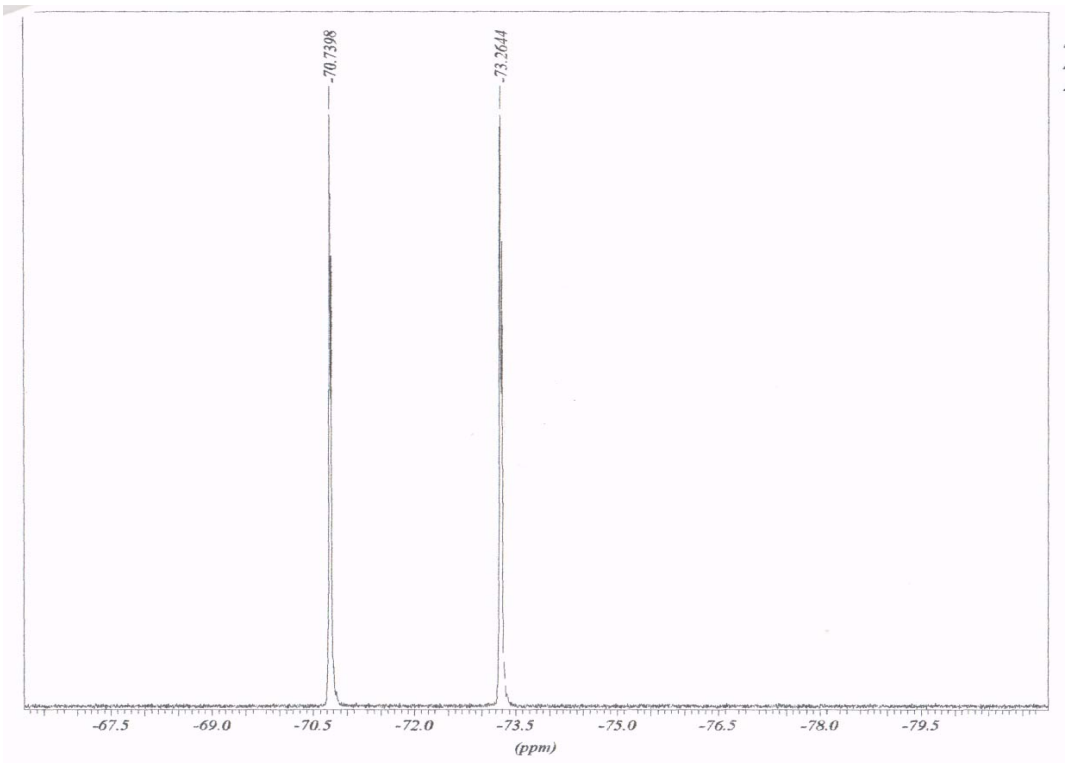
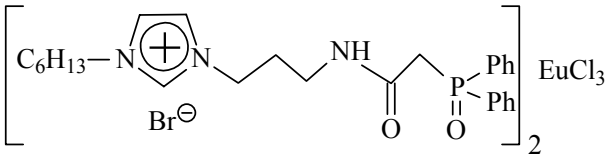


Fig S9. The ^{19}F spectrum for ligand **6f**



7a

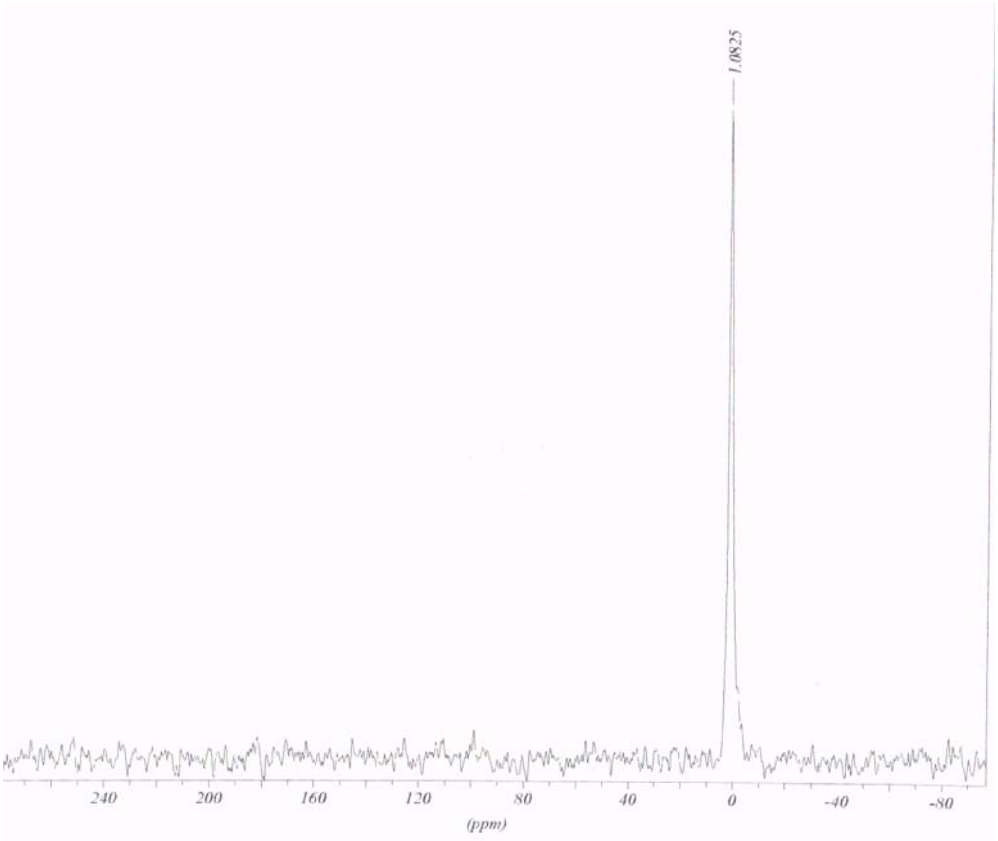


Fig S10. The ^{19}F spectrum for complex **7a**