Supporting Information for

An Electrospray-Active N-Heterocyclic Carbene Ligand for Real-Time Analysis of Organometallic Reactions

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Other supporting information for this manuscript include the following:

X-ray data for [**ESIMes**H]$^{2+}$•2[PF$_6$]$^{-}$: ckjsm2302.cif

Experimental

General Procedures

All glassware used for this work was cleaned by immersion in an acid bath, a base bath, and then thoroughly rinsed with deionized water and dried overnight in an oven. All vials, plastic syringes, and needles were obtained commercially and single used. All substrate synthesis reactions were carried out in a fume hood under air, unless otherwise specified. All solutions of **ESIMes** proligand and reagents were prepared with dried, degassed solvents either in a glovebox or using Schlenk techniques. Toluene (Fisher, ACS, 99.8%), triphenylphosphine (Sigma-Aldrich, reagentplus, 99%), 4-bromobut-1-ene (Oakwood, 97%), bromine (Sigma-Aldrich, reagent grade), 1,2-dichloroethane (Caledon, ACS, 99%), triethyl orthoformate (Sigma-Aldrich, 98%), formic acid (Fisher, ACS, 88% solution), 2,4,6-trimethylaniline (Sigma-Aldrich, 98%, and ammonium hexafluorophosphate (Fisher, 99.5%) were obtained commercially and used without further purification. Dichloromethane (Supelco, HPLC grade, stabilizer-free) was dried over 4 Å molecular sieves and degassed before use.

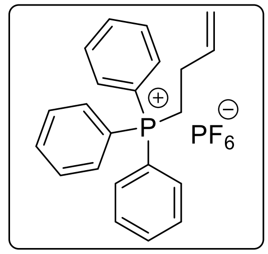
NMR spectra were recorded on a Bruker Avance III 300 Hz NMR spectrometer at standard conditions and referenced to the residual proton or ^{13}C atom of the solvent. NMR chemical shifts are reported in ppm relative to TMS at 0 ppm. $CDCl_3$ (Sigma-Aldrich, 99.8 atom % D) was stored over 4 Å molecular sieves. CD_3CN (Sigma-Aldrich 99.8 atom % D) was purchased in ampoules and used as received. These solvents were used for all ^1H, $^{31}P\{^1H\}$, and $^{13}C\{^1H\}$ NMR spectra.

All kinetic mass spectrometry experiments were performed in dichloromethane and conducted with a Waters Synapt G2-Si in positive mode with a capillary voltage of 3.00 kV and a cone voltage of 15 V. Optimal desolvation was obtained using a desolvation gas flow of 100 L h^{-1}, cone gas flow of 100 L h^{-1}, source temperature of 50 °C, and a desolvation gas temperature of 150 °C. Scan time was set to one second, with an inter-scan time of 0.1 seconds.

Experimental Procedure for Kinetics Experiments

Solutions were prepared in a PSI[1] flask in dichloromethane in a glovebox or using Schlenk techniques to a total concentration in **ESIMes** of 10 µM. The PSI flask was sealed with a septum and Young's tap and removed from the glovebox/Schlenk line and heated to 40 °C with stirring. Then, under an overpressure of 5 psi of argon (Praxair Canada, 99.999%), the headspace of the PSI flask was briefly purged by puncturing the septum with a needle. A 60 cm length of PEEK tubing (0.127 mm I.D.) was inserted into the PSI flask through the septum and connected to the source of the mass spectrometer. Upon establishing a stable analyte signal, additional reagents were added *via* syringe. The combination of 5 psi overpressure and ~60 cm of 0.127 mm I.D. PEEK tubing gives a solution flow rate of about 25 µL/min through the source of the instrument.

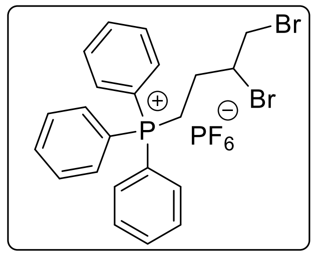
Synthesis of (but-3-enyl)triphenylphosphonium hexafluorophosphate:



To a vial was added triphenylphosphine (3.000 g, 11.44 mmol), 4-bromobut-1-ene (3.089 g, 22.88 mmol), and a stir bar. The resulting mixture was stirred at 95 °C for 24 hours. The resulting precipitate was dissolved in 3 mL of methanol and added slowly to a beaker containing a solution of sodium hexafluorophosphate (1.660 g, 22.88 mmol) in 9 mL of deionized water, forming a flocculant white precipitate. The solid was collected on a sintered glass filter funnel and dried under air. The dry solid was then washed with two 5 mL portions of toluene, and one 5 mL portion of pentane, and dried under high vacuum. The product was obtained as a pure white solid in a 61.5% yield.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 – 7.62 (m, 15H), 5.86 (ddt, *J* = 16.7, 10.1, 6.4 Hz, 1H), 5.16 – 4.98 (m, 2H), 3.33 – 3.17 (m, 2H), 2.47 – 2.32 (m, 2H). ^{31}P{^{1}H} NMR (122 MHz, $CDCl_3$) δ 23.4 (s), -144.3 (sp, *J* = 714.4 Hz). ^{13}C{^{1}H} NMR (76 MHz, $CDCl_3$) δ 134.3 (*J* = 15.6 Hz), 133.4 (*J* = 10.0 Hz), 130.7 (*J* = 12.6 Hz), 117.6 (*J* = 87.4 Hz), 117.7, 135.4 (*J* = 3.0 Hz), 26.4 (*J* = 3.4 Hz), 21.7 (*J* = 51.3 Hz).

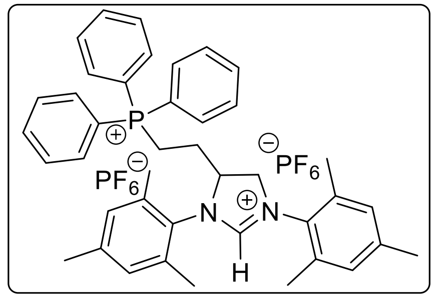
Synthesis of (1,2-dibromobutyl)triphenylphosphonium hexafluorophosphate:



To a 50 mL round-bottom flask was added 1,2-dichloroethane (15 mL), (but-3- enyl)triphenylphosphonium hexafluorophosphate (1.600 g, 3.46 mmol, 0.23 M), and a stir bar. To the resulting solution was then added dropwise a solution of 0.57 M Br_2 in 1,2-dichloroethane (6.82 mL, 1.1 eq.). The mixture immediately took on a yellow colour, with the orange colour of the bromine solution rapidly fading after each drop was added, until taking on an orange colour after complete addition. The mixture was diluted with 30 mL dichloromethane and washed with 10 mL saturated aqueous sodium thiosulfate. The colourless organic layer was then dried with sodium sulfate and filtered, followed by washing the sodium sulfate with 3 x 10 mL dichloromethane. The combined organic layers were concentrated *in vacuo* to give 2.612 g of the product (1,2-dibromobutyl)triphenylphosphonium hexafluorophosphate as a white solid in an 96.5% yield.

^{1}H NMR (300 MHz, CD_3CN) δ 7.97 – 7.81 (m, 3H), 7.82 – 7.67 (m, 12H), 4.41 (tdd, J = 8.3, 4.9, 3.5 Hz, 1H), 3.93 (ddd, J = 10.8, 4.9, 0.5 Hz, 1H), 3.87 – 3.68 (m, 1H), 3.55 – 3.22 (m, 2H), 2.52 – 2.31 (m, 1H), 2.29 – 2.07 (m, 1H). ^{31}P{^{1}H} NMR (122 MHz, CD_3CN) δ 23.77 (s), -144.63 (sept, *J* = 706.5 Hz). ^{13}C{^{1}H} NMR (76 MHz, CD_3CN) δ 136.4, 134.7, 131.4, 118.6, 52.6, 36.8, 30.0, 21.0.

Synthesis of 1,3-dimesityl-5-(2-(triphenylphosphonio)ethyl)imidazolinium dihexafluorophosphate ([**ESIMes**H^{2+}] dihexafluorophosphate):



To a 4 dram screw-capped vial was added 1.794 g (1,2-dibromobutyl)triphenylphosphonium hexafluorophosphate (2.88 mmol), 2.34 g 2,4,6-trimethylaniline (2.43 mL, 17.3 mmol, 6 eq.), and a stir bar. The mixture was heated to 120 °C and stirred for 28 h, by which point it had solidified into a hard, tacky mass. The resulting mixture was dissolved in portions of dichloromethane totalling 60 mL, and the combined solution was washed with 50 mL each of 15% aqueous NaOH and saturated aqueous sodium chloride. The organic layer was dried with anhydrous sodium sulfate and filtered, washing the sodium sulfate with small portions of dichloromethane until they remained colourless. The combined organic solution was concentrated *in vacuo*, giving a thick brown-red oil, which was transferred to a 25 mL round-bottomed flask. To the crude product was twice added 10 mL heptane, which was heated to a boil with vigorous stirring, cooled, and decanted to remove excess 2,4,6-trimethylaniline. The crude residue was used in the next step without further purification.

To the 25 mL flask containing the crude residue from the previous step was added 4.8 mL triethyl orthoformate (10 eq. on starting dibromide), 0.470 g ammonium hexafluorophosphate (1 eq. on starting dibromide), and 0.2 mL formic acid. The mixture was heated to 120 °C and stirred under nitrogen for 3.5 h, after which all volatiles were removed *in vacuo* and the crude product mixture was dissolved in 50 mL dichloromethane. This solution was washed with 20 mL 5% $NaHCO_3$, 20 mL water, 10 mL saturated aqueous sodium chloride, and dried with anhydrous sodium sulfate. After concentration *in vacuo*, the crude brown solid was purified by crystallization from 1,2-dichloroethane:hexane, giving 1.607 g of a white solid in a 63.0% yield on (1,2-dibromobutyl)triphenylphosphonium hexafluorophosphate.

^{1}H NMR (300 MHz, CD_3CN) δ 8.16 (s, 1H), 7.95 – 7.84 (m, 3H), 7.77 – 7.57 (m, 12H), 7.09 (s, 3H), 6.99 (t, *J* = 1.5 Hz, 1H), 4.95 (qd, *J* = 9.1, 4.2 Hz, 1H), 4.65 (t, *J* = 11.9 Hz, 1H), 4.16 (dd, *J* = 12.5, 8.9 Hz, 1H), 3.36 – 3.15 (m, 1H), 2.95 – 2.75 (m, 1H), 2.39 – 2.28 (m, 12H), 2.25 (s, 3H), 2.05 (s, 3H). ^{31}P{^{1}H} NMR (122 MHz, CD_3CN) δ 23.67, -141.70 (sept, *J* = 706.8 Hz). ^{13}C{^{1}H} NMR (76 MHz, CD_3CN) δ 160.4, 142.0, 137.0, 136.7, 136.5, 134.6, 131.5, 131.0, 130.8, 129.5, 118.7, 118.34, 117.5, 64.7, 56.8, 26.3, 21.1, 21.0, 19.4, 18.68, 18.30, 17.92. ESI(+)-MS Calc'd for $C_{41}H_{45}N_2P$: 298.1655, found: 298.1669 (Δ 4.7 ppm).

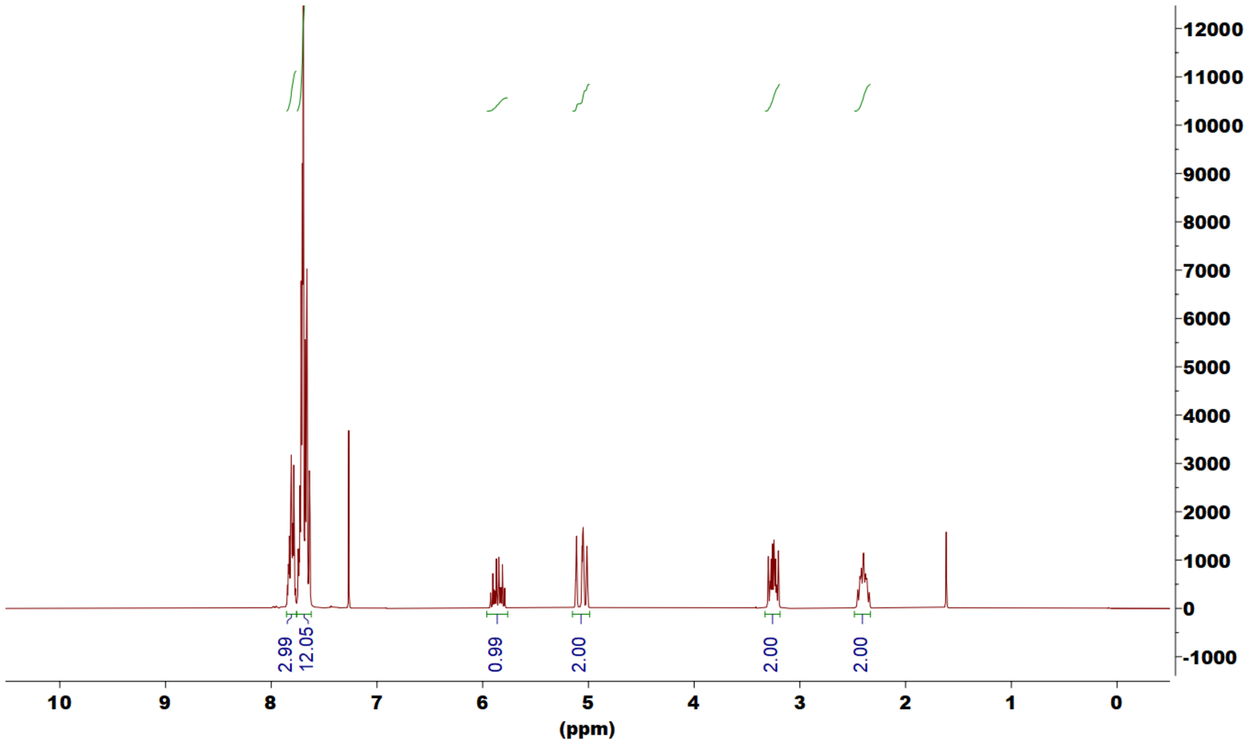


Figure S1. ^{1}H NMR spectrum of (but-3-enyl)triphenylphosphonium hexafluorophosphate.

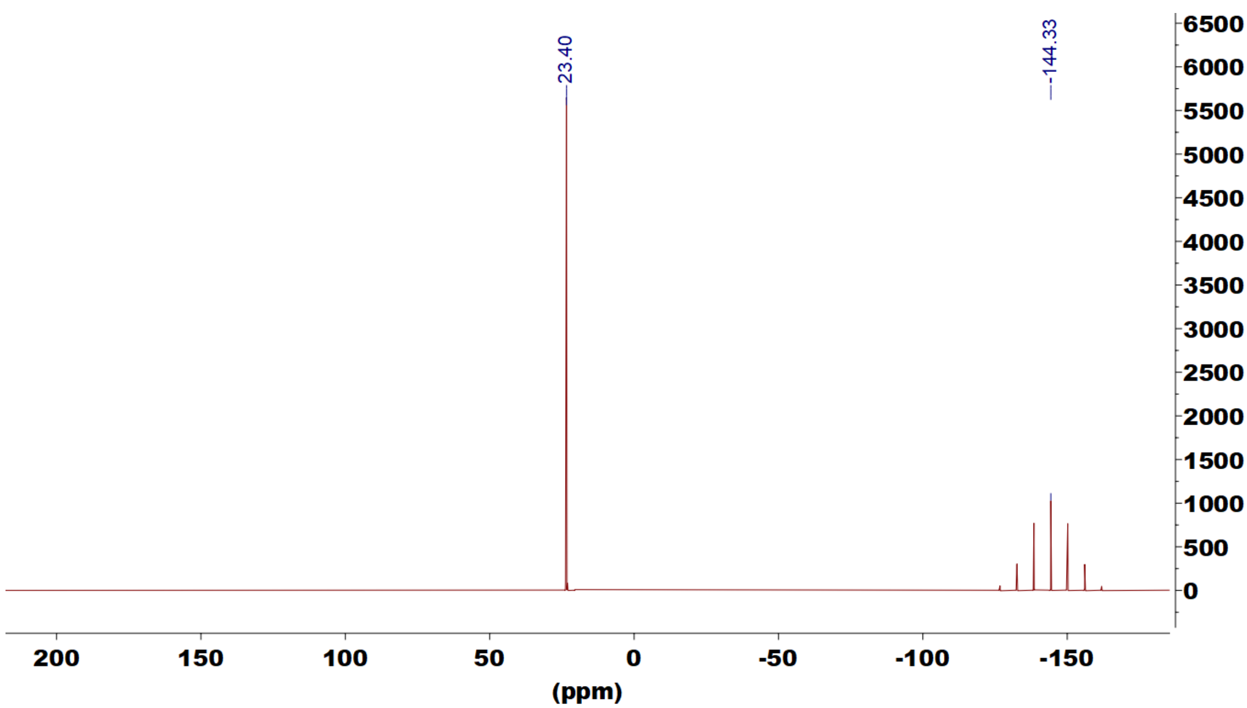


Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum of (but-3-enyl)triphenylphosphonium hexafluorophosphate.

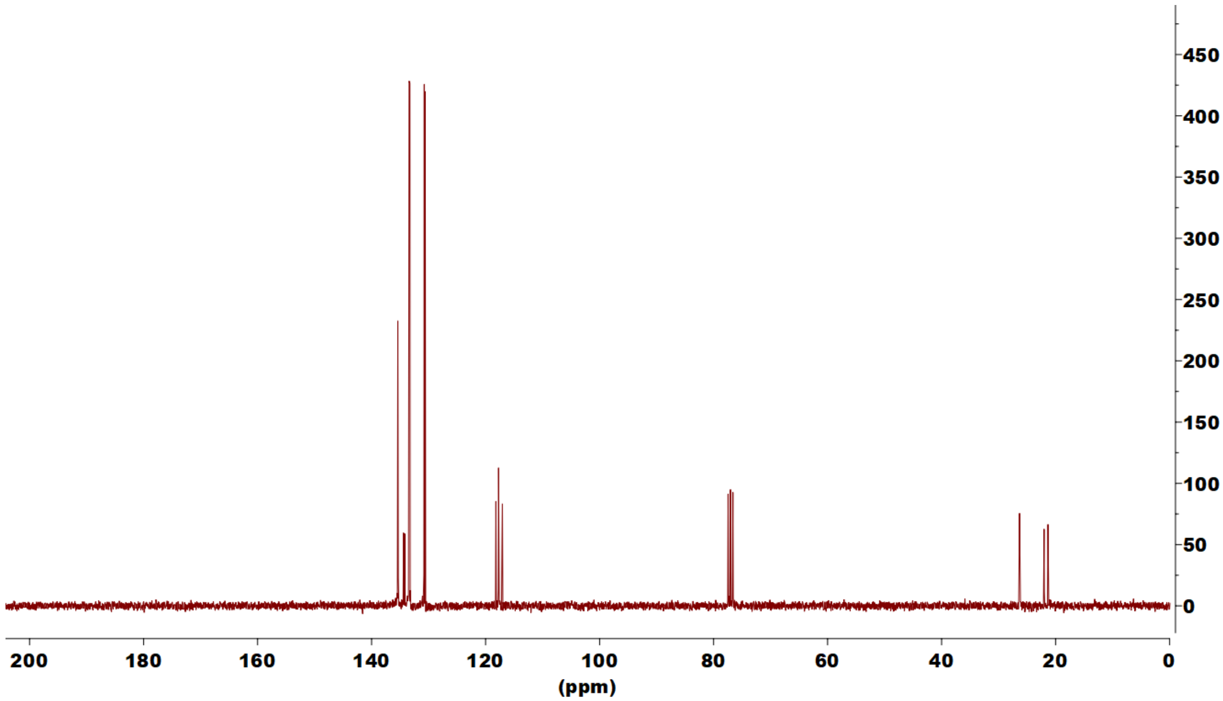


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of (but-3-enyl)triphenylphosphonium hexafluorophosphate.

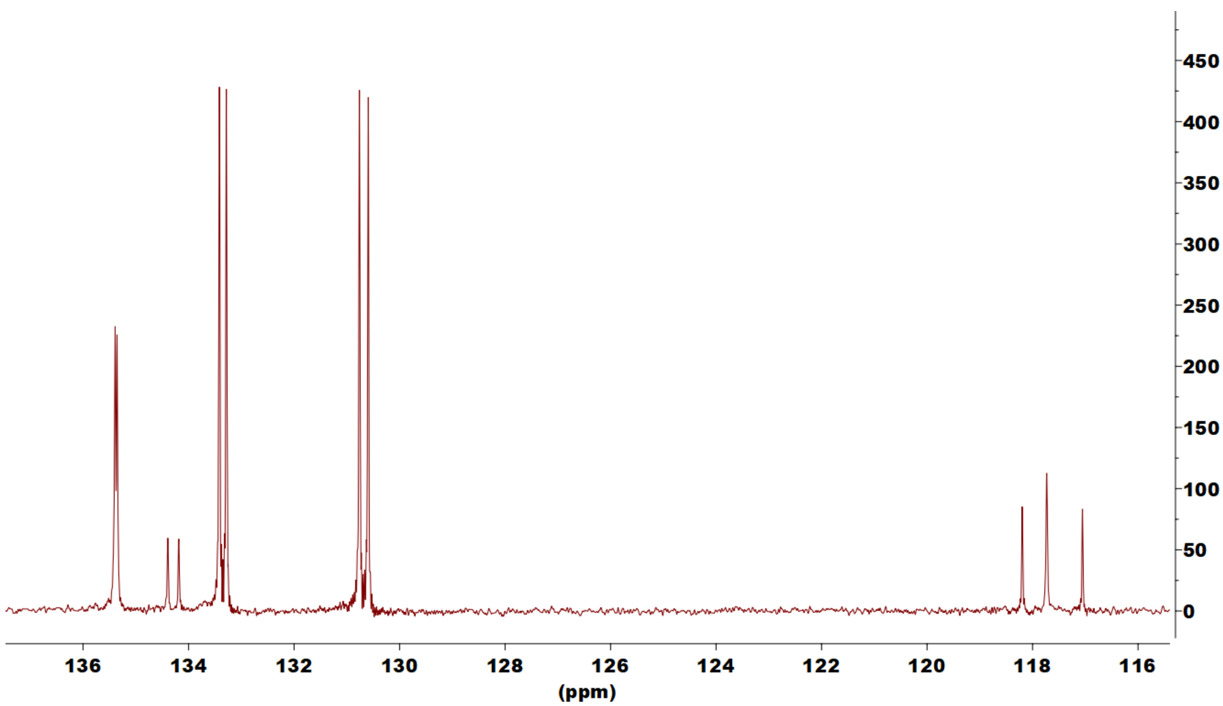


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of (but-3-enyl)triphenylphosphonium hexafluorophosphate (sp^2 region).

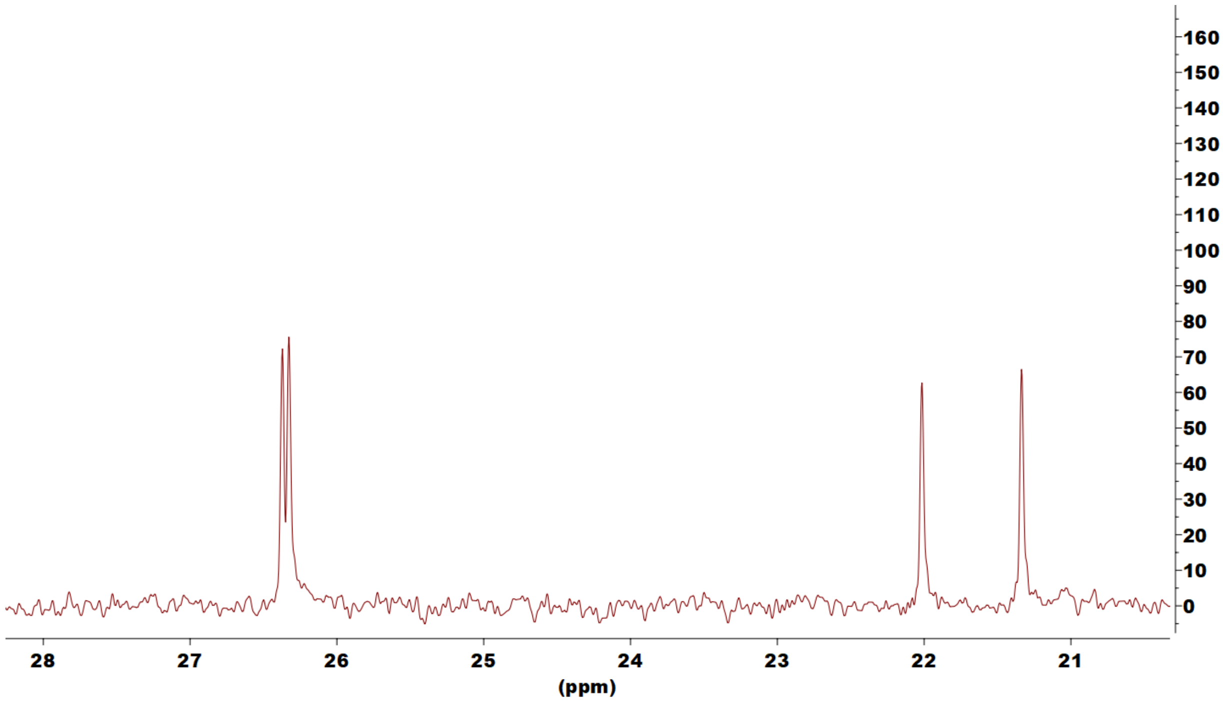


Figure S5. $^{13}C\{^1H\}$ NMR spectrum of (but-3-enyl)triphenylphosphonium hexafluorophosphate (sp^3 region).

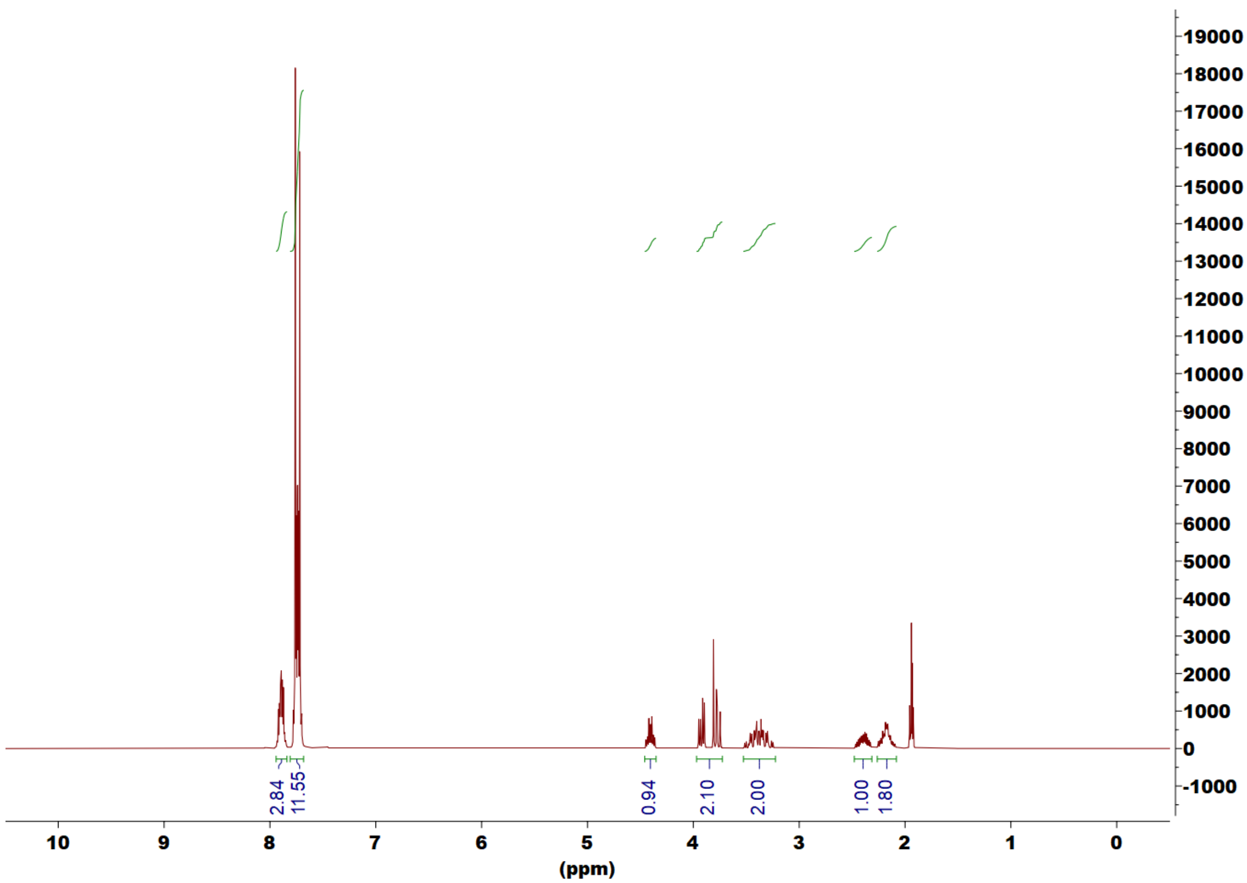


Figure S6. ^1H NMR spectrum of (1,2-dibromobutyl)triphenylphosphonium hexafluorophosphate.

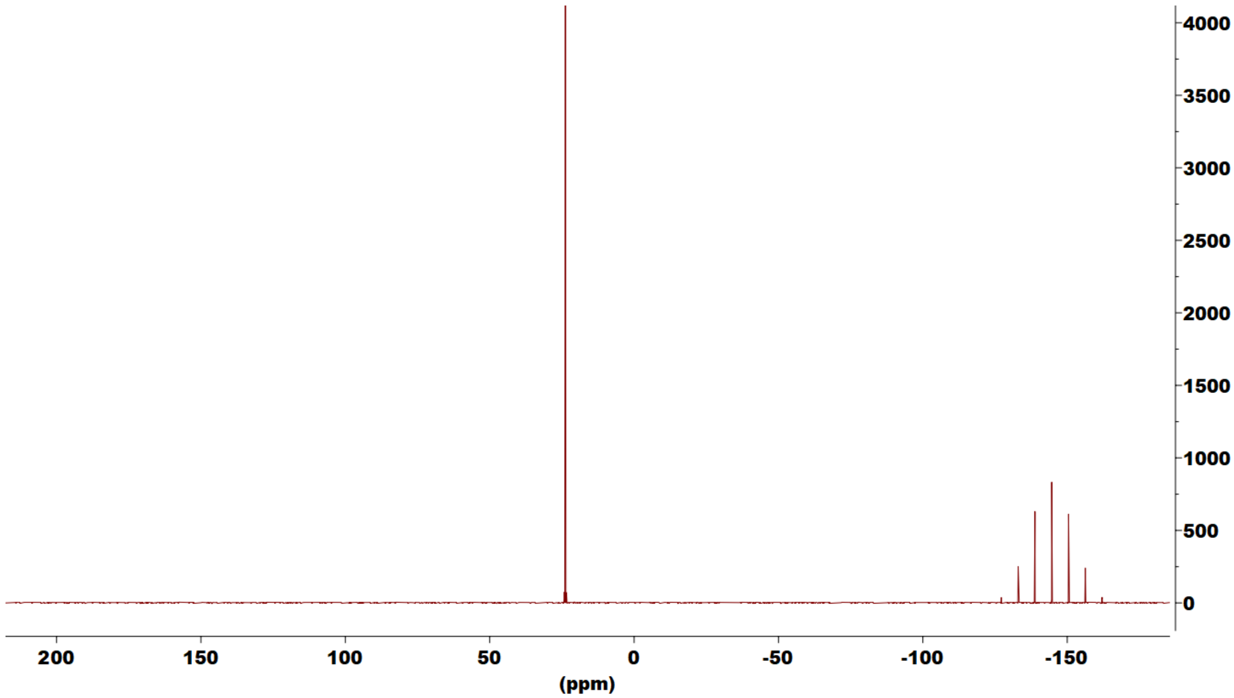


Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum of (1,2-dibromobutyl)triphenylphosphonium hexafluorophosphate.

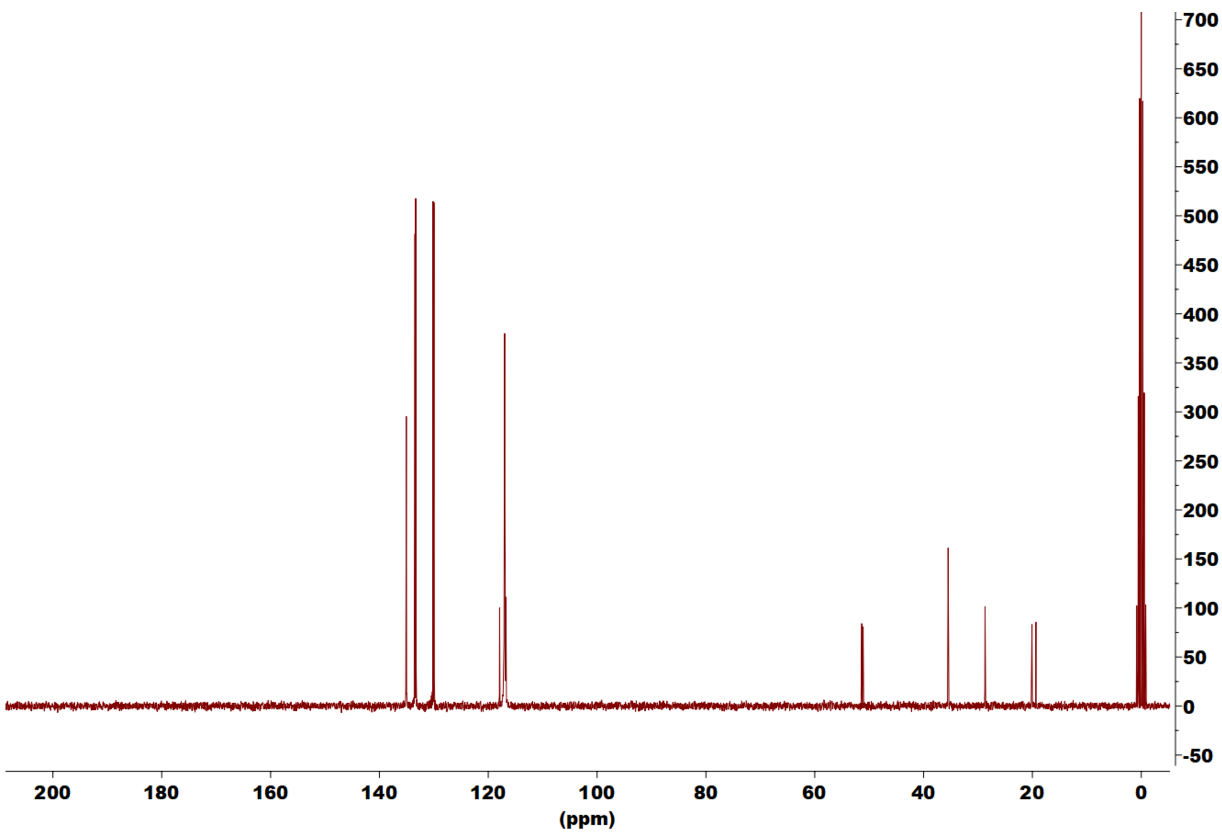


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of (1,2-dibromobutyl)triphenylphosphonium hexafluorophosphate.

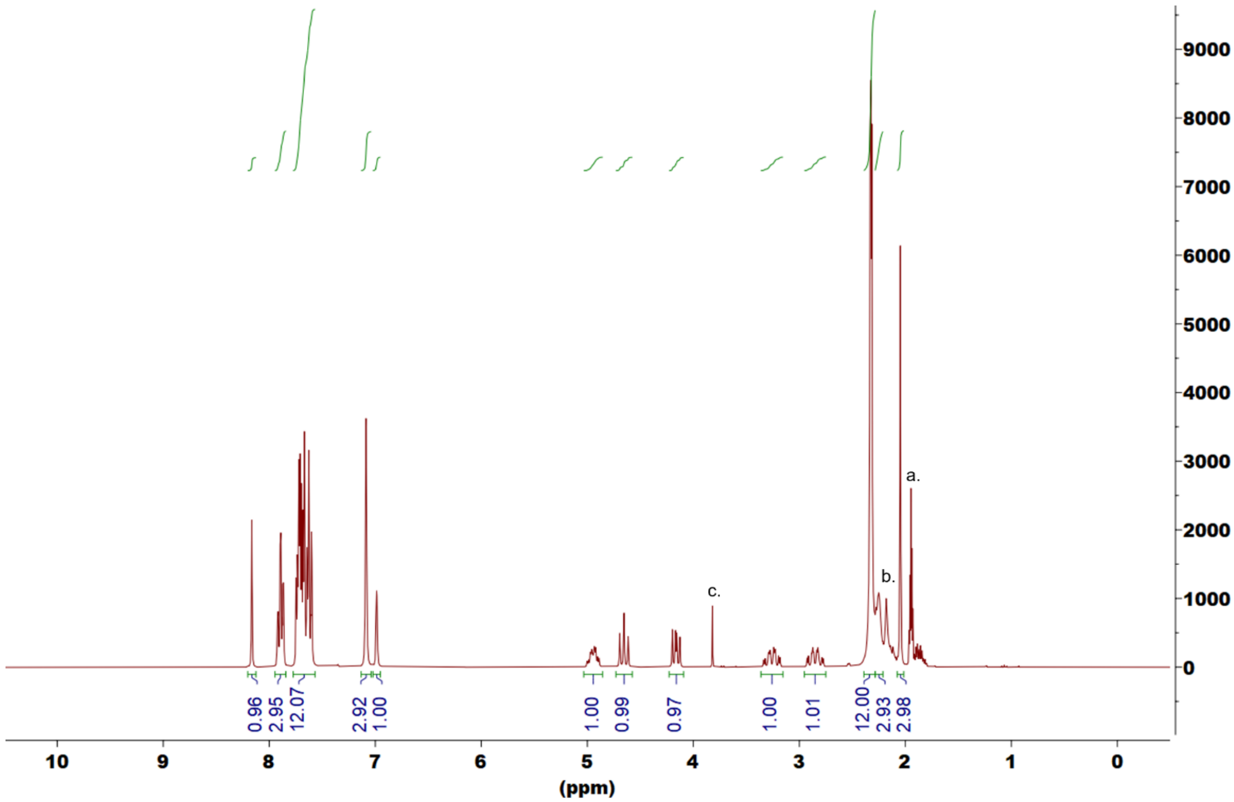


Figure S9. ^{1}H NMR spectrum of **ESIMes**H^{2+} dihexafluorophosphate. Labelled impurities are a. CD_2HCN, b. HDO, c. 1,2-dichloroethane.

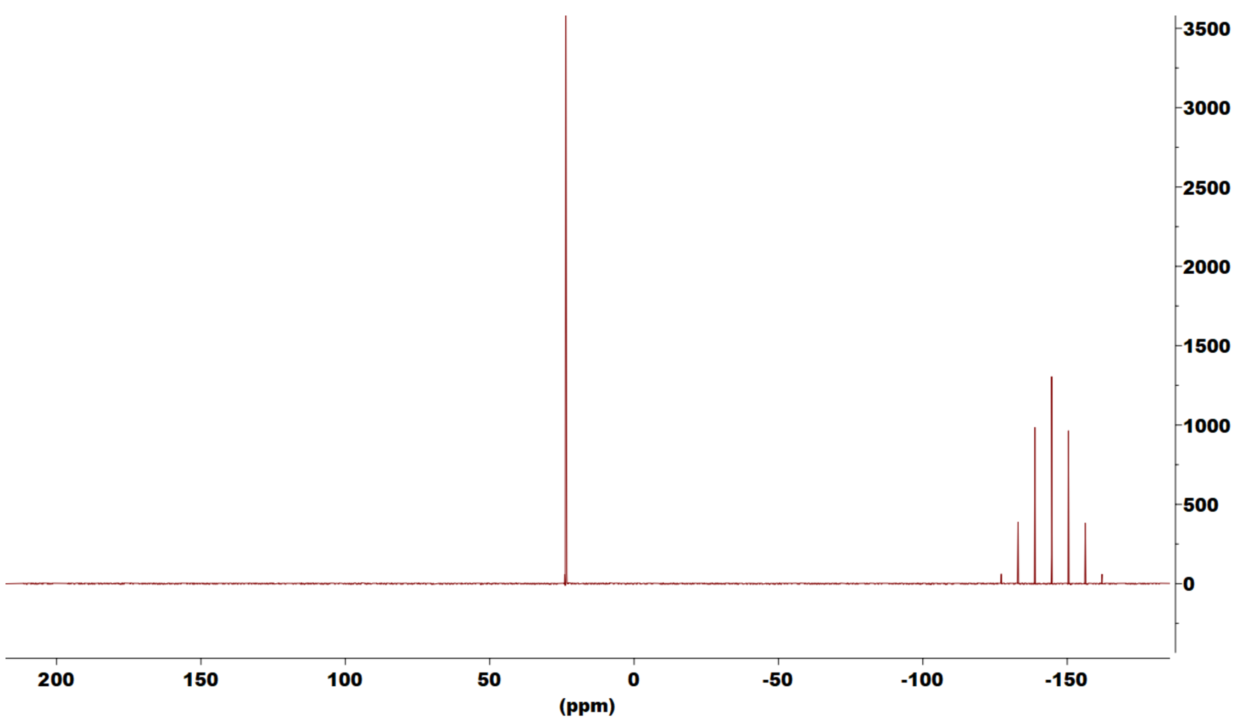


Figure S10. $^{31}P\{^{1}H\}$ NMR spectrum of **ESIMes**H^{2+} dihexafluorophosphate.

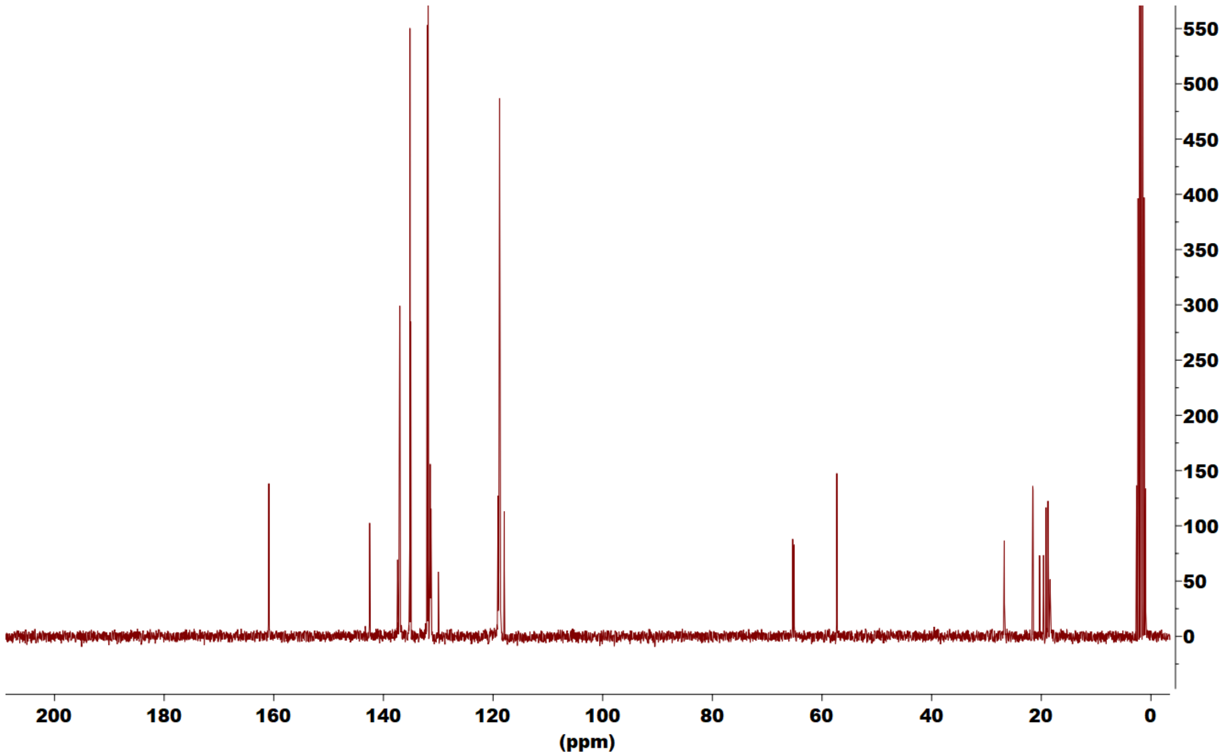


Figure S11. $^{13}C\{^1H\}$ NMR spectrum of **ESIMes**H^{2+} dihexafluorophosphate.

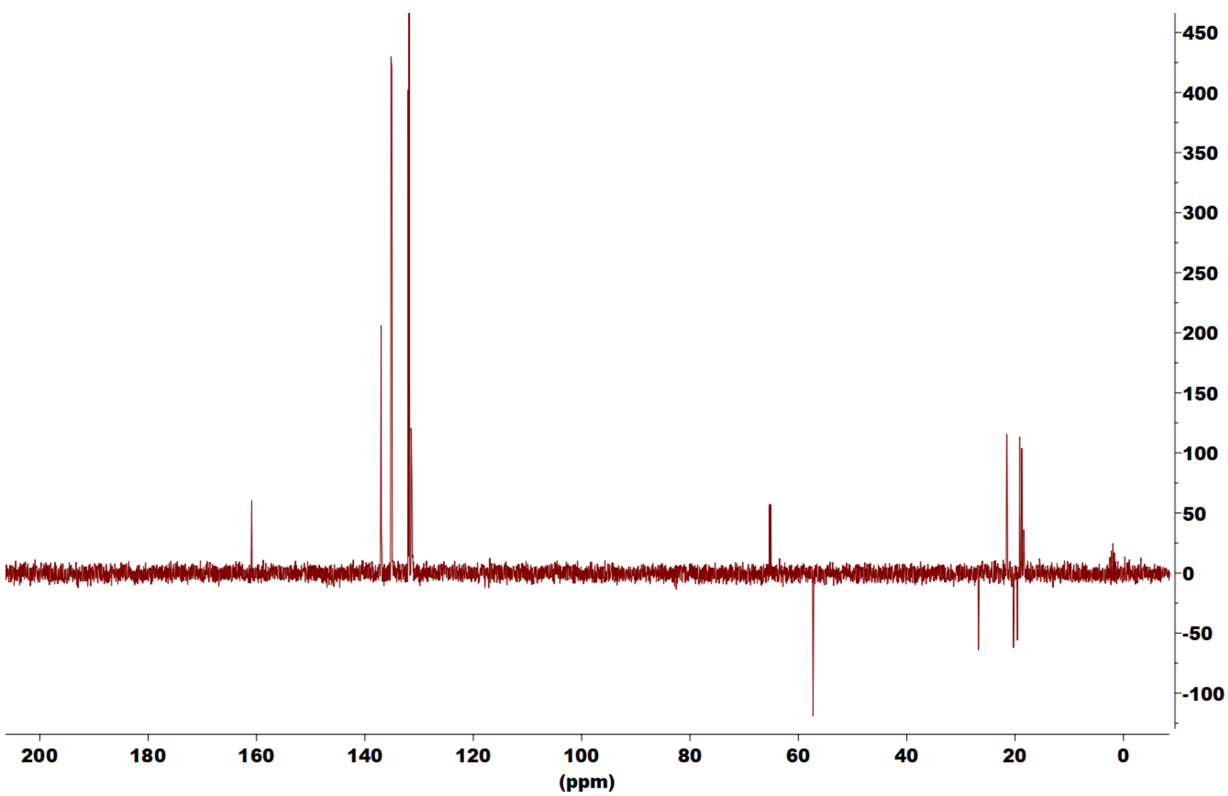


Figure S12. $^{13}C\{^1H\}$ (DEPT-135) NMR spectrum of **ESIMes**H^{2+} dihexafluorophosphate.

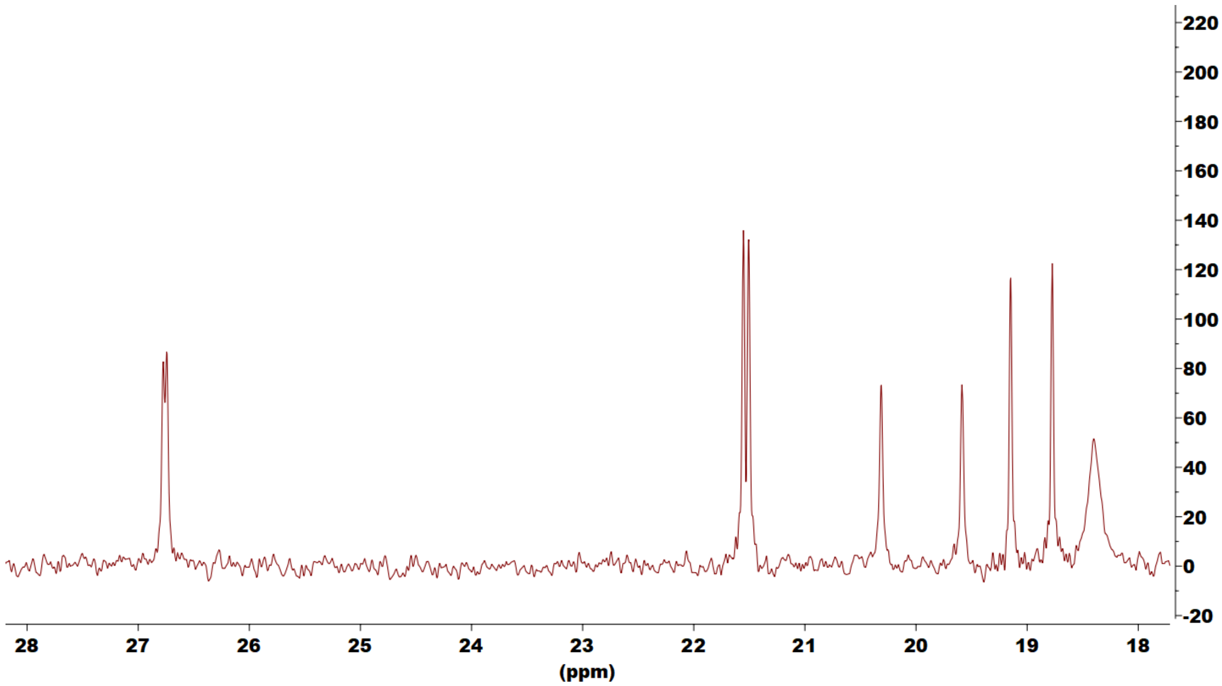


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of **ESIMes**H^{2+} dihexafluorophosphate (sp^3 region).

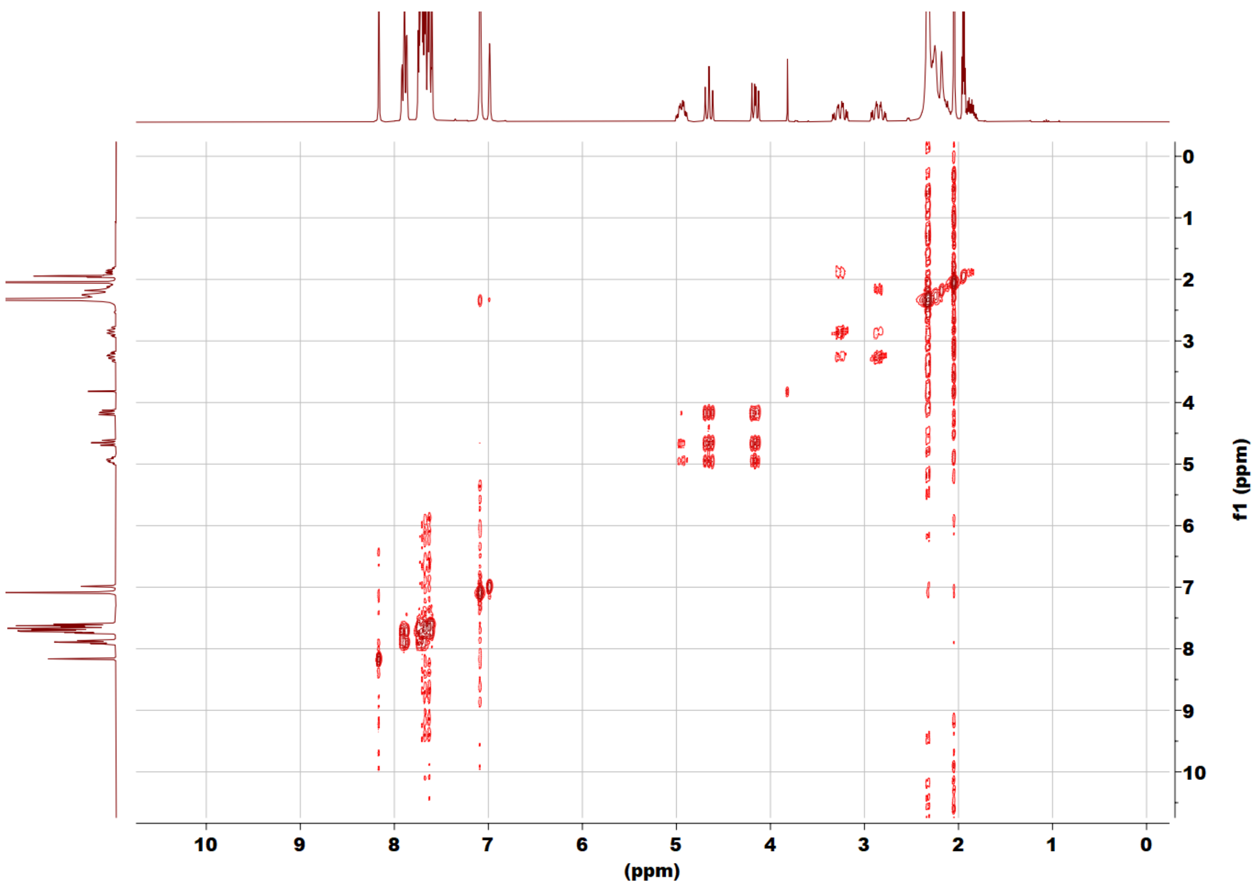


Figure S14. ^{1}H-^{1}H COSY NMR spectrum of **ESIMes**H^{2+} dihexafluorophosphate.

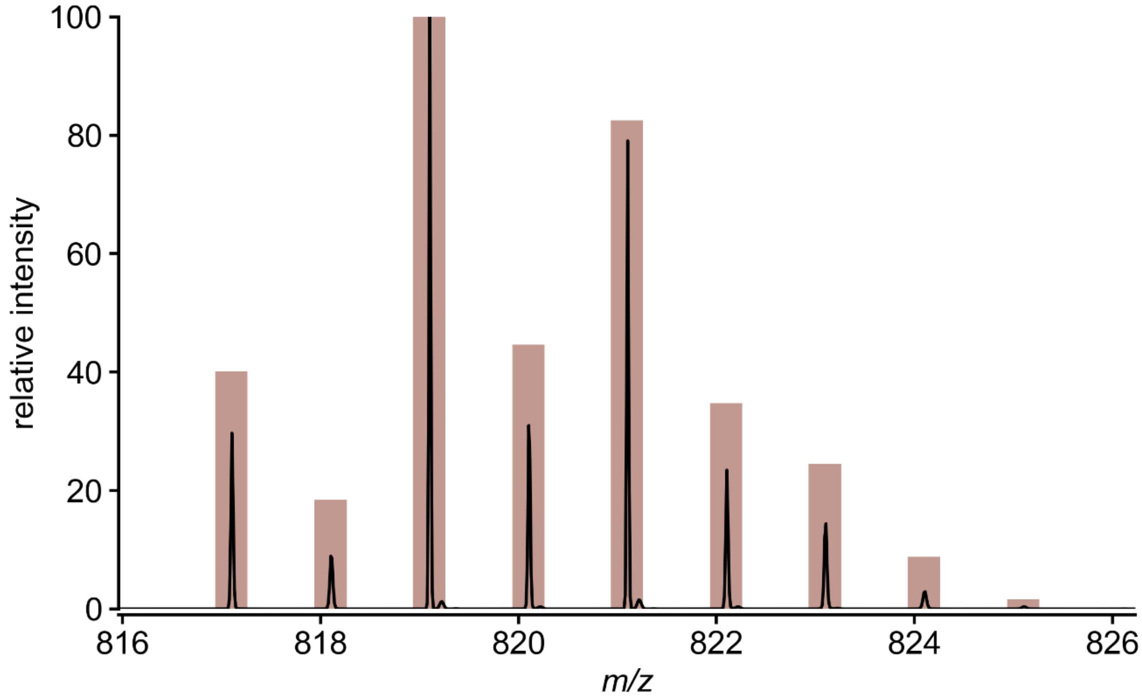


Figure S15. ESI(+) MS spectrum with calculated overlay of [**ESIMes**H]$^{2+}$ [$CuBr_2$]$^{-}$.

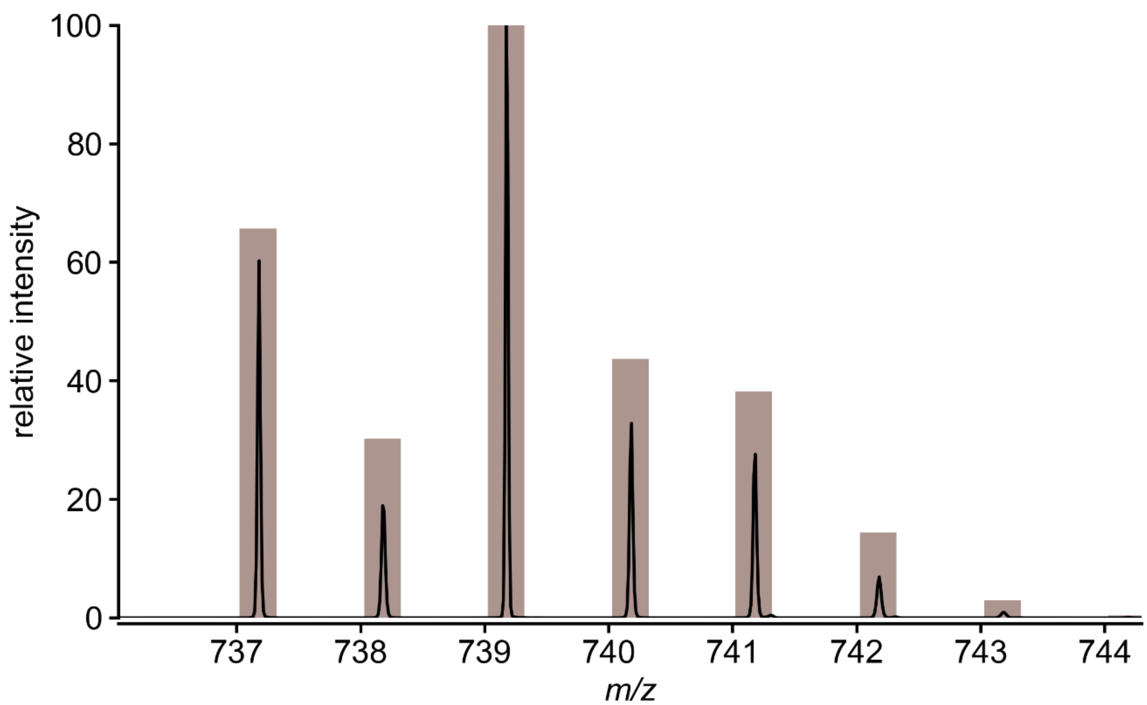


Figure S16. ESI(+) MS spectrum with calculated overlay of [**ESIMes**-CuBr]$^{+}$.

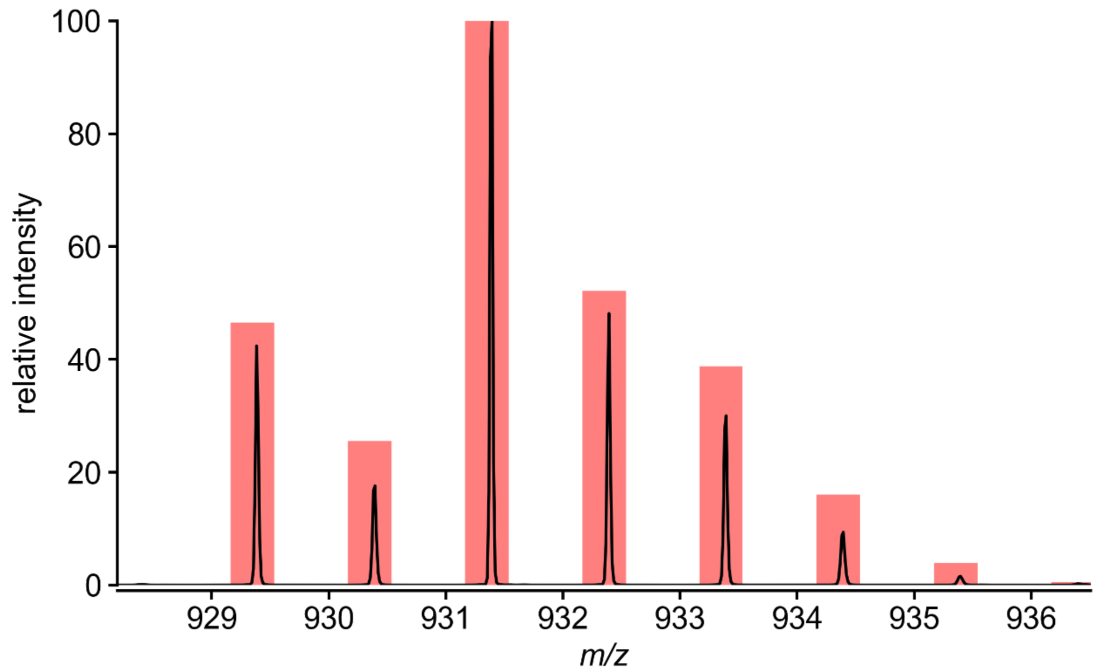


Figure S17. ESI(+) MS spectrum with calculated overlay of [**ESIMes**Ir(cod)Cl]$^+$.

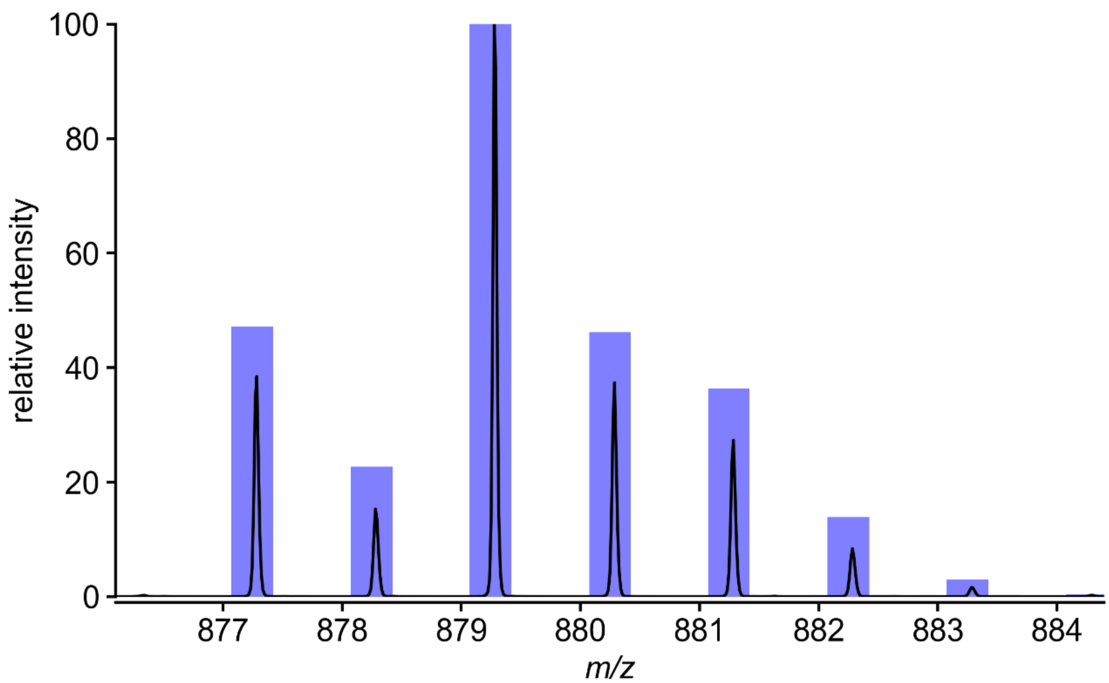


Figure S18. ESI(+) MS spectrum with calculated overlay of [**ESIMes**Ir$(CO)_2$Cl]$^+$.

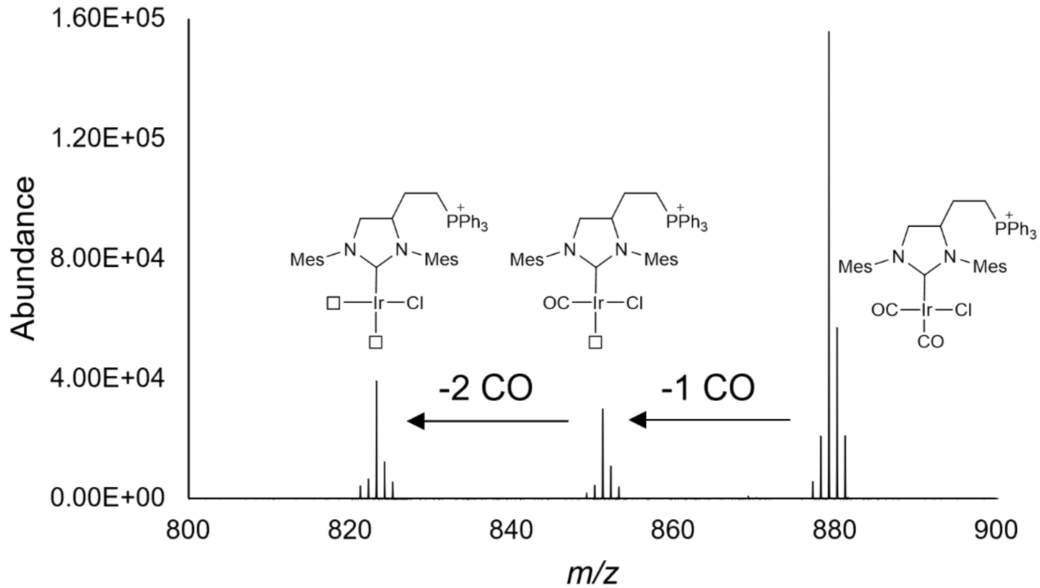


Figure S19. ESI(+) MS/MS spectrum of [**ESIMes**Ir$(CO)_2$Cl]$^+$ at 10 V collision voltage, showing loss of one and two carbonyl ligands.

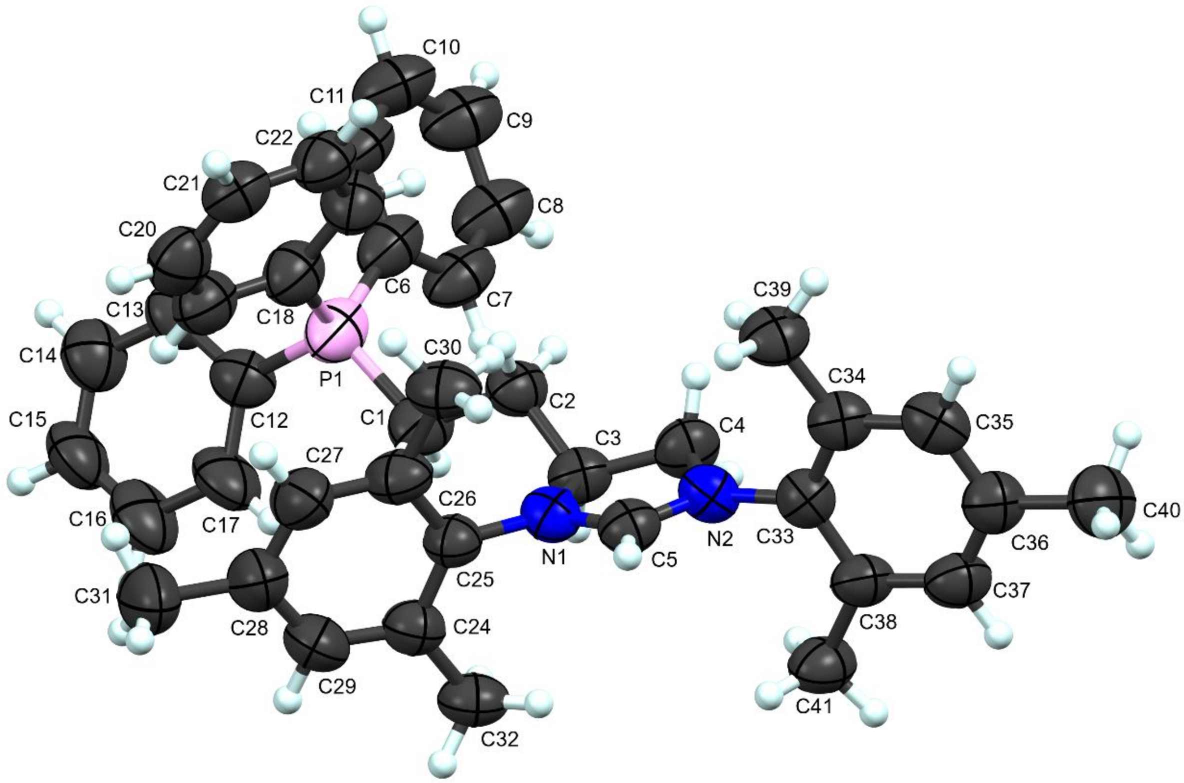


Figure S20. X-ray crystal structure (with disorder removed) of the **ESIMes**H^{2+} cation.

<u>DISCUSSION</u>

The NHC phosphine hexafluorophosphate salt crystallizes as colourless, rod-like crystals. There are two crystallographically independent, yet chemically identical, NHC phosphine di-cations, four PF_6 anions and three, half-occupancy water molecules of crystallization in the unit cell of the primitive, acentric, monoclinic space group $P2_1$. Although the molecule is achiral, it crystallizes in a chiral space group. This leads to a racemic twin (inversion twin) of ~0.605:0.395 ratio.

The overall structure of the salt is as expected (see Figure). The molecules exhibit disorder in both of the independent phosphines. In one (P1) the disorder is a simple flip or slide of one phenyl ring. In the second phosphine (P2) the disorder extends from one phenyl ring through the phosphorus into the ethylene chain. In both cases the atoms were modeled at half occupancy with phenyl rings constrained to an ideal hexagon. Similarity restraints were applied to the displacement parameters of the disordered atoms. There is some exaggerated displacement of the PF_6 fluorine atoms, however, further modeling of this was not warranted because it did not improve the model or impart new, meaningful information about the PF_6 anion. The water molecules were found to be partial occupancy and represent a best estimate model.

Bond distances and angles within the molecules are in the expected ranges.

CRYSTAL SUMMARY

Crystal data for $C_{82}H_{93}F_{24}N_4O_{1.50}P_6$; M_r = 1800.42; Monoclinic; space group $P2_1$; *a* = 9.5558(5) Å; *b* = 21.0574(12) Å; *c* = 21.9139(14) Å; α = 90°; β = 99.961(3)°; γ = 90°; V = 4343.1(4) $Å^3$; Z = 2; T = 120(2) K; λ(Cu-Kα) = 1.54178 Å; μ(Cu-Kα) = 2.018 mm^{-1}; d_{calc} = 1.377 $g.cm^{-3}$; 95092 reflections collected; 16012 unique (R_{int} = 0.0813); giving R_1 = 0.0740, wR_2 = 0.2048 for 12073 data with [I>2σ(I)] and R_1 = 0.0918, wR_2 = 0.2280 for all 16012 data. Residual electron density ($e^-.Å^{-3}$) max/min: 0.460/-0.535.

An arbitrary sphere of data was collected on a colourless rod-like crystal, having approximate dimensions of 0.187 × 0.058 × 0.054 mm, on a Bruker Venture diffractometer equipped with a Bruker PHOTON-III detector using a combination of ω- and φ-scans of 0.5°.[1] Data were corrected for absorption and polarization effects and analyzed for space group determination [2]. The structure was solved by dual-space methods and expanded routinely [3]. The model was refined by full-matrix least-squares analysis of F^2 against all reflections [4]. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. Unless otherwise noted, hydrogen atoms were included in calculated positions. Atomic displacement parameters for the hydrogens were tied to the equivalent isotropic displacement parameter of the atom to which they are bonded (U_{iso}(H) = 1.5U_{eq}(C) for methyl, 1.2U_{eq}(C) for all others).

Table 1. Crystal data and structure refinement for ckjsm2302.

Identification code	ckjsm2302
Empirical formula	$C_{82}H_{93}F_{24}N_4O_{1.50}P_6$
Formula weight	1800.42
Temperature (K)	120(2)
Wavelength (Å)	1.54178
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	
a (Å)	9.5558(5)
b (Å)	21.0574(12)
c (Å)	21.9139(14)
α (°)	90
β (°)	99.961(3)
γ (°)	90
Volume (Å^3)	4343.1(4)
Z	2
Density (calc; g.cm^{-3})	1.377
Absorption coefficient (μ mm^{-1})	2.018
F(000)	1862
Crystal color, habit	colourless, rod
Crystal size (mm^3)	0.187 × 0.058 × 0.054
θ range for data collection (°)	2.047 to 68.871
Index ranges	-9 ≤ h ≤ 11, -25 ≤ k ≤ 25, -26 ≤ l ≤ 26
Reflections collected	95092
Independent reflections	16012 [R_{int} = 0.0813]
Completeness to θ = 67.679°	100.0 %
Absorption correction	Numerical
Max. and min. transmission	0.8643 and 0.5902
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16012 / 187 / 1172
Goodness-of-fit on F^2	1.032
Final R indices [I>2σ(I)]	R_1 = 0.0740, wR_2 = 0.2048
R indices (all data)	R_1 = 0.0918, wR_2 = 0.2280
Absolute structure parameter	0.40(4)
Extinction coefficient	n/a
Largest diff. peak and hole (e$^-$.Å^{-3})	0.460 and -0.535

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for ckjsm2302. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
P(1)	0.3254(3)	0.61554(11)	0.53780(12)	0.087(1)
N(1)	0.6200(6)	0.4580(3)	0.4606(3)	0.065(1)
N(2)	0.6279(6)	0.4387(3)	0.3626(3)	0.066(1)
C(1)	0.3698(9)	0.5398(4)	0.5080(4)	0.083(2)
C(2)	0.4265(8)	0.5429(4)	0.4468(4)	0.073(2)
C(3)	0.4744(7)	0.4763(3)	0.4283(4)	0.065(2)
C(4)	0.4890(8)	0.4712(4)	0.3599(4)	0.075(2)
C(5)	0.6935(7)	0.4348(3)	0.4199(4)	0.066(2)
C(6)	0.2015(9)	0.6565(4)	0.4831(5)	0.083(2)
C(7)	0.0952(9)	0.6238(4)	0.4426(5)	0.086(2)
C(8)	-0.0093(10)	0.6563(5)	0.4049(6)	0.097(3)
C(9)	-0.0153(11)	0.7210(5)	0.4050(6)	0.101(3)
C(10)	0.0885(12)	0.7550(5)	0.4437(6)	0.106(3)
C(11)	0.1941(13)	0.7234(5)	0.4825(6)	0.102(3)
C(12)	0.2279(16)	0.6046(7)	0.5982(7)	0.074(5)
C(13)	0.1653(18)	0.6561(6)	0.6225(9)	0.078(5)
C(14)	0.1092(18)	0.6492(7)	0.6766(9)	0.093(6)
C(15)	0.1157(18)	0.5907(8)	0.7063(7)	0.094(7)
C(16)	0.1782(18)	0.5391(6)	0.6819(7)	0.104(6)
C(17)	0.2344(17)	0.5460(6)	0.6279(7)	0.097(5)
C(12A)	0.2695(18)	0.5950(10)	0.6124(8)	0.093(7)
C(13A)	0.1582(19)	0.6306(10)	0.6278(9)	0.102(7)
C(14A)	0.1015(17)	0.6152(11)	0.6802(9)	0.104(7)
C(15A)	0.1561(19)	0.5643(11)	0.7172(7)	0.121(10)
C(16A)	0.267(2)	0.5287(8)	0.7017(8)	0.120(7)
C(17A)	0.3242(18)	0.5441(8)	0.6493(8)	0.101(6)
C(18)	0.4843(9)	0.6597(4)	0.5599(4)	0.083(2)
C(19)	0.5590(11)	0.6600(5)	0.6224(5)	0.090(2)
C(20)	0.6863(11)	0.6910(5)	0.6357(5)	0.091(2)
C(21)	0.7455(9)	0.7222(4)	0.5912(5)	0.082(2)
C(22)	0.6731(10)	0.7230(4)	0.5295(4)	0.083(2)
C(23)	0.5424(9)	0.6916(4)	0.5140(4)	0.081(2)
C(24)	0.6664(8)	0.4618(3)	0.5266(3)	0.065(2)
C(25)	0.7535(9)	0.5125(4)	0.5505(4)	0.077(2)
C(26)	0.7821(11)	0.5187(5)	0.6141(4)	0.088(2)
C(27)	0.7315(13)	0.4774(5)	0.6539(4)	0.094(3)
C(28)	0.6506(12)	0.4264(4)	0.6270(4)	0.089(2)
C(29)	0.6172(8)	0.4158(4)	0.5644(4)	0.073(2)
C(30)	0.8156(9)	0.5577(4)	0.5096(5)	0.086(2)
C(31)	0.7631(17)	0.4879(6)	0.7239(5)	0.120(4)
C(32)	0.5350(9)	0.3589(4)	0.5389(5)	0.080(2)
C(33)	0.6795(7)	0.4160(4)	0.3084(3)	0.064(2)
C(34)	0.7550(6)	0.4572(4)	0.2765(4)	0.066(2)
C(35)	0.7937(7)	0.4362(4)	0.2218(4)	0.072(2)
C(36)	0.7595(8)	0.3752(4)	0.2010(4)	0.074(2)
C(37)	0.6884(8)	0.3343(4)	0.2344(4)	0.076(2)

C(38)	0.6476(8)	0.3536(3)	0.2891(4)	0.069(2)
C(39)	0.7959(8)	0.5231(4)	0.3011(4)	0.079(2)
C(40)	0.7993(12)	0.3538(6)	0.1387(5)	0.098(3)
C(41)	0.5676(10)	0.3095(4)	0.3257(5)	0.084(2)
P(2)	0.6909(7)	0.7861(3)	0.1080(3)	0.063(1)
C(42)	0.6648(13)	0.7042(6)	0.1321(9)	0.061(3)
C(43)	0.5088(15)	0.6940(7)	0.1003(9)	0.064(4)
P(2A)	0.7216(7)	0.7871(3)	0.1362(3)	0.063(2)
C(43A)	0.560(2)	0.6747(9)	0.1333(11)	0.076(4)
C(42A)	0.6177(19)	0.7080(8)	0.0825(12)	0.086(5)
N(3)	0.3390(6)	0.6094(3)	0.0723(4)	0.084(2)
N(4)	0.3491(6)	0.5426(4)	0.1496(4)	0.082(2)
C(44)	0.4880(8)	0.6160(5)	0.1034(5)	0.096(3)
C(45)	0.4842(8)	0.5778(6)	0.1636(5)	0.102(3)
C(46)	0.2755(7)	0.5644(4)	0.0987(4)	0.078(2)
C(47)	0.7801(9)	0.8130(4)	0.0573(6)	0.095(3)
C(48)	0.7570(11)	0.7816(7)	0.0012(8)	0.127(5)
C(49)	0.8108(14)	0.8038(9)	-0.0495(7)	0.139(6)
C(50)	0.8914(11)	0.8600(8)	-0.0418(5)	0.117(4)
C(51)	0.9127(8)	0.8922(5)	0.0132(5)	0.089(2)
C(52)	0.8586(9)	0.8690(4)	0.0639(5)	0.083(2)
C(53)	0.5548(10)	0.8344(4)	0.1286(5)	0.089(3)
C(54)	0.4929(12)	0.8736(4)	0.0804(6)	0.097(3)
C(55)	0.3665(12)	0.9058(5)	0.0861(6)	0.101(3)
C(56)	0.3036(10)	0.8974(5)	0.1374(5)	0.093(3)
C(57)	0.3664(12)	0.8591(5)	0.1856(6)	0.101(3)
C(58)	0.4937(11)	0.8280(4)	0.1820(5)	0.092(3)
C(59)	0.8226(10)	0.7834(6)	0.1745(6)	0.064(4)
C(60)	0.8429(13)	0.8340(6)	0.2158(7)	0.071(5)
C(61)	0.9594(15)	0.8346(7)	0.2635(7)	0.091(6)
C(62)	1.0556(14)	0.7845(8)	0.2701(7)	0.102(9)
C(63)	1.0353(14)	0.7339(7)	0.2288(7)	0.089(6)
C(64)	0.9189(13)	0.7333(6)	0.1810(6)	0.076(4)
C(63A)	1.0841(14)	0.7613(8)	0.2570(9)	0.101(9)
C(62A)	1.0886(18)	0.8134(9)	0.2963(8)	0.110(9)
C(61A)	0.979(2)	0.8578(8)	0.2873(8)	0.143(13)
C(60A)	0.8655(17)	0.8501(7)	0.2390(9)	0.108(10)
C(59A)	0.8610(13)	0.7980(7)	0.1997(7)	0.069(5)
C(64A)	0.9703(14)	0.7537(7)	0.2087(8)	0.078(5)
C(65)	0.2781(8)	0.6340(4)	0.0103(5)	0.083(2)
C(66)	0.3041(9)	0.6009(4)	-0.0410(6)	0.092(3)
C(67)	0.2403(11)	0.6225(4)	-0.0986(6)	0.095(3)
C(68)	0.1496(12)	0.6753(4)	-0.1056(6)	0.101(3)
C(69)	0.1283(14)	0.7069(4)	-0.0530(7)	0.118(4)
C(70)	0.1947(12)	0.6870(4)	0.0072(7)	0.112(4)
C(71)	0.3956(11)	0.5420(5)	-0.0358(6)	0.112(4)
C(72)	0.0711(15)	0.6932(6)	-0.1687(6)	0.123(4)
C(73)	0.1659(16)	0.7239(6)	0.0635(7)	0.135(5)
C(74)	0.3038(6)	0.4920(5)	0.1852(4)	0.082(2)
C(75)	0.3438(8)	0.4306(5)	0.1720(5)	0.091(3)
C(76)	0.2913(10)	0.3793(6)	0.2037(6)	0.105(3)

C(77)	0.2023(9)	0.3892(7)	0.2443(6)	0.105(4)
C(78)	0.1646(8)	0.4530(7)	0.2579(5)	0.106(4)
C(79)	0.2143(7)	0.5051(5)	0.2279(5)	0.091(3)
C(80)	0.4331(9)	0.4184(6)	0.1226(6)	0.100(3)
C(81)	0.1432(11)	0.3338(8)	0.2763(7)	0.129(5)
C(82)	0.1704(8)	0.5721(6)	0.2405(5)	0.099(3)
P(3)	1.0875(3)	0.39210(13)	0.4685(3)	0.137(2)
F(1)	1.1202(10)	0.3253(5)	0.4994(9)	0.260(9)
F(2)	0.9803(7)	0.3610(4)	0.4176(6)	0.169(4)
F(3)	0.9601(6)	0.3996(3)	0.5082(4)	0.132(3)
F(4)	1.1957(9)	0.4193(7)	0.5207(6)	0.212(7)
F(5)	1.2110(6)	0.3801(4)	0.4271(5)	0.152(4)
F(6)	1.0531(10)	0.4590(3)	0.4387(4)	0.148(3)
P(4)	0.5168(2)	0.69663(12)	0.32205(11)	0.081(1)
F(7)	0.5040(8)	0.6212(3)	0.3142(4)	0.127(2)
F(8)	0.4082(6)	0.7031(3)	0.2587(2)	0.093(1)
F(9)	0.3898(6)	0.6940(4)	0.3605(3)	0.108(2)
F(10)	0.6267(7)	0.6874(7)	0.3836(3)	0.177(5)
F(11)	0.6429(6)	0.6981(4)	0.2840(3)	0.114(2)
F(12)	0.5216(13)	0.7704(4)	0.3282(4)	0.166(4)
P(5)	0.3971(4)	0.1640(2)	0.17656(16)	0.122(1)
F(13)	0.4350(19)	0.1008(7)	0.1481(7)	0.257(8)
F(14)	0.2598(12)	0.1709(6)	0.1248(4)	0.167(4)
F(15)	0.3072(14)	0.1270(4)	0.2172(5)	0.172(4)
F(16)	0.5325(13)	0.1665(7)	0.2268(6)	0.211(5)
F(17)	0.4786(14)	0.2046(9)	0.1350(6)	0.240(8)
F(18)	0.3470(15)	0.2258(5)	0.2058(6)	0.186(4)
P(6)	0.86411(17)	0.54961(11)	0.06488(10)	0.073(1)
F(19)	0.9741(4)	0.5024(2)	0.1052(2)	0.080(1)
F(20)	0.7727(9)	0.4931(3)	0.0398(5)	0.184(5)
F(21)	0.7804(6)	0.5574(4)	0.1201(3)	0.124(2)
F(22)	0.9579(7)	0.6092(3)	0.0954(4)	0.126(2)
F(23)	0.9614(7)	0.5496(4)	0.0140(3)	0.128(2)
F(24)	0.7575(5)	0.5976(3)	0.0245(3)	0.096(2)
O(1)	0.0895(16)	0.0371(6)	0.1214(6)	0.094(4)
O(2)	-0.102(2)	-0.0210(8)	0.1743(9)	0.142(8)
O(3)	0.601(2)	-0.0004(11)	0.1887(12)	0.156(8)
H(1A)	0.44225	0.51905	0.53949	0.100
H(1B)	0.28397	0.51260	0.50201	0.100
H(2A)	0.50793	0.57256	0.45116	0.087
H(2B)	0.35124	0.55924	0.41375	0.087
H(3)	0.40455	0.44385	0.43751	0.078
H(4A)	0.41070	0.44576	0.33626	0.091
H(4B)	0.48967	0.51372	0.34066	0.091
H(5)	0.78551	0.41685	0.43123	0.079
H(7)	0.09627	0.57868	0.44138	0.103
H(8)	-0.07998	0.63328	0.37798	0.117
H(9)	-0.08974	0.74263	0.37873	0.121
H(10)	0.08659	0.80011	0.44334	0.127
H(11)	0.26364	0.74709	0.50939	0.123
H(13)	0.16092	0.69613	0.60218	0.094

H(14)	0.06646	0.68447	0.69320	0.112
H(15)	0.07733	0.58597	0.74324	0.113
H(16)	0.18266	0.49913	0.70226	0.124
H(17)	0.27712	0.51079	0.61125	0.117
H(13A)	0.12081	0.66539	0.60259	0.122
H(14A)	0.02540	0.63952	0.69081	0.124
H(15A)	0.11741	0.55378	0.75301	0.146
H(16A)	0.30484	0.49392	0.72698	0.144
H(17A)	0.40025	0.51978	0.63876	0.121
H(19)	0.52068	0.63899	0.65421	0.108
H(20)	0.73582	0.69098	0.67719	0.109
H(21)	0.83441	0.74312	0.60200	0.099
H(22)	0.71267	0.74474	0.49850	0.099
H(23)	0.49331	0.69189	0.47243	0.097
H(26)	0.83955	0.55330	0.63138	0.106
H(28)	0.61632	0.39697	0.65379	0.107
H(30A)	0.89971	0.53847	0.49709	0.129
H(30B)	0.84278	0.59718	0.53220	0.129
H(30C)	0.74493	0.56697	0.47263	0.129
H(31A)	0.84859	0.46409	0.74176	0.181
H(31B)	0.68249	0.47304	0.74228	0.181
H(31C)	0.77854	0.53322	0.73259	0.181
H(32A)	0.43466	0.37030	0.52670	0.121
H(32B)	0.54434	0.32554	0.57053	0.121
H(32C)	0.57192	0.34334	0.50261	0.121
H(35)	0.84363	0.46364	0.19861	0.087
H(37)	0.66729	0.29234	0.21968	0.091
H(39A)	0.71396	0.54321	0.31453	0.119
H(39B)	0.82600	0.54868	0.26830	0.119
H(39C)	0.87425	0.51992	0.33629	0.119
H(40A)	0.78977	0.38977	0.10989	0.148
H(40B)	0.73559	0.31948	0.12099	0.148
H(40C)	0.89764	0.33853	0.14565	0.148
H(41A)	0.62530	0.30137	0.36645	0.126
H(41B)	0.54815	0.26928	0.30331	0.126
H(41C)	0.47769	0.32933	0.33099	0.126
H(42A)	0.73021	0.67432	0.11630	0.073
H(42B)	0.67614	0.70030	0.17769	0.073
H(43A)	0.49342	0.70910	0.05686	0.076
H(43B)	0.44239	0.71640	0.12289	0.076
H(43C)	0.49135	0.70205	0.14997	0.092
H(43D)	0.63782	0.66312	0.16755	0.092
H(42C)	0.54126	0.72236	0.04899	0.104
H(42D)	0.68614	0.68122	0.06491	0.104
H(44)	0.55215	0.59442	0.07838	0.115
H(44A)	0.55195	0.59428	0.07839	0.115
H(45A)	0.56597	0.54834	0.17254	0.122
H(45B)	0.48513	0.60647	0.19944	0.122
H(46)	0.18330	0.54915	0.08191	0.094
H(48)	0.70267	0.74358	-0.00279	0.152
H(49)	0.79392	0.78202	-0.08803	0.167

H(50)	0.93186	0.87596	-0.07541	0.141
H(51)	0.96497	0.93077	0.01689	0.107
H(52)	0.87501	0.89106	0.10233	0.100
H(54)	0.53486	0.87864	0.04439	0.117
H(55)	0.32427	0.93374	0.05410	0.121
H(56)	0.21627	0.91798	0.13965	0.112
H(57)	0.32312	0.85406	0.22118	0.122
H(58)	0.53859	0.80253	0.21554	0.110
H(60)	0.77716	0.86827	0.21132	0.085
H(61)	0.97325	0.86923	0.29175	0.109
H(62)	1.13522	0.78493	0.30271	0.122
H(63)	1.10110	0.69968	0.23323	0.107
H(64)	0.90500	0.69872	0.15280	0.091
H(63A)	1.15886	0.73102	0.26320	0.121
H(62A)	1.16637	0.81863	0.32937	0.132
H(61A)	0.98230	0.89333	0.31416	0.171
H(60A)	0.79074	0.88040	0.23279	0.130
H(64A)	0.96730	0.71809	0.18182	0.094
H(67)	0.25841	0.60088	-0.13447	0.114
H(69)	0.06770	0.74301	-0.05699	0.141
H(71A)	0.48840	0.55133	-0.01059	0.168
H(71B)	0.40871	0.52858	-0.07730	0.168
H(71C)	0.34922	0.50796	-0.01631	0.168
H(72A)	0.13933	0.70566	-0.19513	0.184
H(72B)	0.00707	0.72875	-0.16493	0.184
H(72C)	0.01564	0.65670	-0.18720	0.184
H(73A)	0.09377	0.70160	0.08217	0.202
H(73B)	0.13165	0.76651	0.05072	0.202
H(73C)	0.25386	0.72720	0.09386	0.202
H(76)	0.31933	0.33713	0.19605	0.126
H(78)	0.10497	0.46006	0.28768	0.128
H(80A)	0.38457	0.43554	0.08294	0.149
H(80B)	0.44693	0.37259	0.11858	0.149
H(80C)	0.52563	0.43920	0.13421	0.149
H(81A)	0.03994	0.33179	0.26306	0.193
H(81B)	0.16532	0.33976	0.32125	0.193
H(81C)	0.18622	0.29419	0.26508	0.193
H(82A)	0.25432	0.59972	0.24686	0.148
H(82B)	0.12652	0.57258	0.27772	0.148
H(82C)	0.10202	0.58758	0.20506	0.148
H(1OA)	0.15809	0.01180	0.11974	0.141
H(1OB)	0.02495	0.01864	0.13705	0.141
H(2OA)	-0.12643	-0.05632	0.18783	0.213
H(2OB)	-0.16763	-0.01201	0.14428	0.213
H(3OA)	0.56670	0.03677	0.18959	0.234
H(3OB)	0.67301	0.00416	0.17127	0.234

Table 3. Anisotropic displacement parameters (Å^2) for ckjsm2302.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P(1)	0.0937(13)	0.0789(12)	0.0997(16)	-0.0136(11)	0.0498(12)	-0.0193(11)
N(1)	0.058(3)	0.068(3)	0.069(3)	0.005(3)	0.013(2)	-0.006(2)
N(2)	0.055(3)	0.074(4)	0.069(4)	0.009(3)	0.013(2)	0.006(2)
C(1)	0.085(5)	0.077(5)	0.098(6)	-0.004(4)	0.043(4)	-0.013(4)
C(2)	0.078(4)	0.065(4)	0.082(5)	0.004(4)	0.033(4)	-0.003(3)
C(3)	0.051(3)	0.062(4)	0.083(5)	0.002(3)	0.017(3)	-0.002(3)
C(4)	0.067(4)	0.072(4)	0.089(5)	-0.001(4)	0.017(3)	0.011(3)
C(5)	0.058(3)	0.063(4)	0.079(5)	0.000(3)	0.016(3)	-0.008(3)
C(6)	0.081(5)	0.069(4)	0.112(6)	-0.021(4)	0.051(5)	-0.017(4)
C(7)	0.079(5)	0.066(4)	0.125(7)	-0.018(4)	0.049(5)	-0.019(4)
C(8)	0.071(4)	0.079(5)	0.152(9)	-0.015(6)	0.048(5)	-0.013(4)
C(9)	0.085(5)	0.080(5)	0.149(9)	-0.004(6)	0.050(6)	-0.010(4)
C(10)	0.101(6)	0.063(5)	0.160(11)	-0.009(6)	0.044(7)	-0.003(5)
C(11)	0.117(7)	0.068(5)	0.132(9)	-0.025(5)	0.051(7)	-0.021(5)
C(12)	0.063(9)	0.078(10)	0.082(11)	0.009(8)	0.016(9)	-0.005(8)
C(13)	0.070(10)	0.094(12)	0.076(10)	0.012(9)	0.030(8)	0.003(9)
C(14)	0.086(11)	0.111(15)	0.089(12)	0.000(12)	0.033(9)	-0.011(11)
C(15)	0.109(14)	0.113(16)	0.067(12)	0.019(11)	0.031(11)	-0.020(12)
C(16)	0.107(12)	0.131(15)	0.081(12)	0.018(11)	0.037(10)	-0.036(13)
C(17)	0.116(13)	0.102(12)	0.080(11)	0.025(9)	0.031(10)	-0.032(11)
C(12A)	0.079(13)	0.116(16)	0.090(13)	-0.015(12)	0.028(11)	-0.008(11)
C(13A)	0.071(10)	0.164(19)	0.077(12)	-0.018(13)	0.029(9)	-0.035(13)
C(14A)	0.078(10)	0.17(2)	0.073(13)	-0.014(16)	0.029(9)	-0.021(14)
C(15A)	0.125(17)	0.16(2)	0.089(15)	-0.010(16)	0.039(14)	-0.046(17)
C(16A)	0.132(16)	0.132(16)	0.105(14)	-0.004(12)	0.048(13)	-0.040(14)
C(17A)	0.109(12)	0.108(13)	0.098(13)	-0.009(11)	0.053(11)	-0.036(12)
C(18)	0.085(5)	0.080(5)	0.091(6)	-0.012(4)	0.037(4)	-0.011(4)
C(19)	0.100(6)	0.079(5)	0.098(6)	-0.008(5)	0.038(5)	-0.008(5)
C(20)	0.093(5)	0.086(5)	0.095(6)	-0.012(5)	0.020(5)	0.013(5)
C(21)	0.079(4)	0.067(4)	0.101(6)	-0.008(4)	0.019(4)	-0.001(4)
C(22)	0.088(5)	0.071(4)	0.094(6)	-0.008(4)	0.028(4)	-0.013(4)
C(23)	0.080(4)	0.083(5)	0.082(5)	-0.005(4)	0.022(4)	-0.016(4)
C(24)	0.069(4)	0.058(3)	0.070(4)	0.001(3)	0.016(3)	-0.008(3)
C(25)	0.076(4)	0.060(4)	0.093(6)	0.002(4)	0.007(4)	-0.013(3)
C(26)	0.102(6)	0.075(5)	0.082(6)	-0.003(4)	0.002(4)	-0.013(4)
C(27)	0.127(7)	0.079(5)	0.075(5)	0.000(4)	0.010(5)	-0.005(5)
C(28)	0.115(6)	0.077(5)	0.079(5)	0.015(4)	0.026(5)	-0.007(5)
C(29)	0.076(4)	0.066(4)	0.077(5)	0.008(3)	0.017(4)	-0.002(3)
C(30)	0.077(4)	0.071(5)	0.109(6)	0.012(4)	0.012(4)	-0.014(4)
C(31)	0.174(12)	0.106(8)	0.076(6)	-0.005(5)	0.006(7)	-0.027(8)
C(32)	0.081(4)	0.064(4)	0.098(6)	0.014(4)	0.021(4)	-0.007(3)
C(33)	0.055(3)	0.071(4)	0.067(4)	0.002(3)	0.011(3)	0.002(3)
C(34)	0.046(3)	0.069(4)	0.084(5)	0.002(3)	0.015(3)	0.000(3)
C(35)	0.048(3)	0.086(5)	0.084(5)	0.016(4)	0.015(3)	0.000(3)
C(36)	0.063(4)	0.077(5)	0.086(5)	0.001(4)	0.024(3)	0.004(3)

C(37)	0.075(4)	0.060(4)	0.097(6)	0.004(4)	0.027(4)	0.006(3)
C(38)	0.070(4)	0.055(3)	0.086(5)	0.005(3)	0.024(3)	0.003(3)
C(39)	0.068(4)	0.074(5)	0.099(6)	0.002(4)	0.023(4)	-0.015(3)
C(40)	0.099(6)	0.108(7)	0.100(7)	0.001(5)	0.050(5)	0.006(5)
C(41)	0.093(5)	0.066(4)	0.100(6)	0.002(4)	0.040(5)	-0.007(4)
P(2)	0.065(3)	0.0459(19)	0.085(4)	0.002(3)	0.033(3)	-0.0018(19)
C(42)	0.045(6)	0.050(7)	0.090(10)	0.003(7)	0.019(6)	-0.003(5)
C(43)	0.053(7)	0.048(7)	0.091(11)	0.016(7)	0.012(7)	0.003(5)
P(2A)	0.072(4)	0.048(2)	0.074(4)	0.005(3)	0.025(3)	-0.001(2)
C(43A)	0.070(9)	0.066(9)	0.103(13)	-0.015(9)	0.042(10)	-0.014(8)
C(42A)	0.072(9)	0.063(9)	0.137(17)	0.022(10)	0.052(11)	0.019(7)
N(3)	0.059(3)	0.062(3)	0.142(6)	0.003(4)	0.045(4)	-0.006(3)
N(4)	0.041(2)	0.090(4)	0.118(5)	0.009(4)	0.019(3)	-0.011(3)
C(44)	0.068(4)	0.094(6)	0.141(8)	-0.044(6)	0.056(5)	-0.033(4)
C(45)	0.048(3)	0.139(8)	0.125(7)	-0.033(7)	0.033(4)	-0.032(4)
C(46)	0.045(3)	0.072(4)	0.123(7)	0.021(4)	0.029(4)	-0.001(3)
C(47)	0.074(4)	0.066(4)	0.158(9)	-0.025(5)	0.054(5)	-0.017(4)
C(48)	0.076(5)	0.131(10)	0.181(13)	-0.075(10)	0.045(7)	-0.010(6)
C(49)	0.094(7)	0.179(14)	0.140(11)	-0.069(11)	0.009(8)	0.028(9)
C(50)	0.073(5)	0.195(14)	0.091(7)	-0.009(8)	0.030(5)	0.038(7)
C(51)	0.065(4)	0.104(6)	0.104(7)	0.010(5)	0.030(4)	-0.011(4)
C(52)	0.077(4)	0.080(5)	0.099(6)	-0.011(4)	0.034(4)	-0.016(4)
C(53)	0.100(6)	0.048(3)	0.137(8)	0.006(4)	0.067(6)	0.005(4)
C(54)	0.110(7)	0.070(5)	0.124(8)	0.008(5)	0.055(6)	0.005(5)
C(55)	0.105(6)	0.084(6)	0.121(8)	0.026(5)	0.040(6)	0.024(5)
C(56)	0.091(5)	0.083(6)	0.112(7)	0.003(5)	0.035(5)	0.024(5)
C(57)	0.116(7)	0.078(5)	0.129(8)	0.021(5)	0.075(7)	0.034(5)
C(58)	0.108(6)	0.059(4)	0.119(7)	0.006(4)	0.051(6)	0.011(4)
C(59)	0.053(9)	0.056(9)	0.087(14)	0.004(8)	0.025(10)	-0.015(7)
C(60)	0.069(9)	0.066(13)	0.077(13)	0.007(12)	0.009(8)	0.002(9)
C(61)	0.068(10)	0.079(14)	0.123(18)	-0.002(13)	0.010(11)	-0.013(9)
C(62)	0.079(15)	0.098(19)	0.12(2)	0.020(17)	0.003(14)	0.002(14)
C(63)	0.093(16)	0.082(14)	0.100(16)	0.011(11)	0.042(13)	0.008(11)
C(64)	0.055(8)	0.066(10)	0.110(14)	0.011(9)	0.019(8)	0.009(7)
C(63A)	0.063(11)	0.099(19)	0.14(2)	0.008(16)	0.011(13)	-0.025(12)
C(62A)	0.091(13)	0.093(16)	0.13(2)	0.013(13)	-0.015(13)	-0.044(12)
C(61A)	0.16(3)	0.071(15)	0.18(3)	-0.030(16)	-0.02(2)	-0.036(16)
C(60A)	0.15(3)	0.073(14)	0.10(2)	-0.016(13)	0.005(18)	-0.033(14)
C(59A)	0.080(11)	0.045(10)	0.078(13)	0.003(8)	-0.001(9)	-0.023(8)
C(64A)	0.062(11)	0.080(14)	0.094(14)	0.003(10)	0.016(10)	-0.023(9)
C(65)	0.069(4)	0.059(4)	0.134(8)	0.014(4)	0.051(5)	0.000(3)
C(66)	0.065(4)	0.060(4)	0.154(9)	-0.013(5)	0.033(5)	-0.006(3)
C(67)	0.094(5)	0.062(4)	0.134(9)	-0.003(5)	0.032(6)	0.007(4)
C(68)	0.104(6)	0.067(5)	0.146(9)	0.023(5)	0.058(7)	0.011(4)
C(69)	0.152(9)	0.058(5)	0.168(11)	0.036(6)	0.096(9)	0.032(5)
C(70)	0.119(7)	0.061(4)	0.181(11)	0.028(6)	0.100(8)	0.025(5)
C(71)	0.085(5)	0.072(5)	0.174(11)	-0.042(6)	0.010(6)	0.020(4)
C(72)	0.136(9)	0.093(7)	0.149(10)	0.040(7)	0.054(8)	0.037(7)
C(73)	0.163(11)	0.095(7)	0.176(12)	0.026(8)	0.114(10)	0.053(8)
C(74)	0.038(3)	0.100(6)	0.106(6)	0.030(5)	0.008(3)	0.001(3)
C(75)	0.053(3)	0.109(7)	0.108(7)	0.024(5)	0.005(4)	-0.001(4)

C(76)	0.071(5)	0.118(8)	0.121(8)	0.035(6)	0.001(5)	0.006(5)
C(77)	0.060(4)	0.137(9)	0.114(8)	0.052(7)	0.000(4)	-0.006(5)
C(78)	0.042(3)	0.169(11)	0.106(7)	0.043(7)	0.005(4)	0.004(5)
C(79)	0.038(3)	0.131(8)	0.103(6)	0.023(6)	0.006(3)	-0.006(4)
C(80)	0.066(4)	0.105(7)	0.130(8)	0.002(6)	0.021(5)	0.011(4)
C(81)	0.081(6)	0.170(12)	0.135(10)	0.081(9)	0.018(6)	0.012(7)
C(82)	0.054(4)	0.131(8)	0.115(7)	0.009(6)	0.025(4)	-0.006(4)
P(3)	0.0635(12)	0.0701(13)	0.269(5)	0.031(2)	0.0094(18)	-0.0003(10)
F(1)	0.145(7)	0.131(7)	0.55(2)	0.171(11)	0.198(11)	0.076(6)
F(2)	0.084(4)	0.144(6)	0.294(12)	-0.112(7)	0.077(5)	-0.039(4)
F(3)	0.084(3)	0.090(4)	0.214(8)	-0.005(4)	0.005(4)	0.023(3)
F(4)	0.105(5)	0.249(12)	0.254(12)	0.134(11)	-0.045(7)	-0.060(6)
F(5)	0.061(3)	0.114(5)	0.281(11)	0.048(6)	0.031(4)	-0.007(3)
F(6)	0.174(7)	0.068(3)	0.180(7)	0.021(4)	-0.033(6)	0.013(4)
P(4)	0.0788(11)	0.0878(13)	0.0816(12)	0.0043(10)	0.0302(10)	-0.0017(10)
F(7)	0.152(5)	0.079(3)	0.163(6)	0.040(4)	0.065(5)	0.029(4)
F(8)	0.097(3)	0.100(4)	0.082(3)	0.013(3)	0.017(2)	0.015(3)
F(9)	0.088(3)	0.151(5)	0.092(3)	0.006(4)	0.037(3)	0.018(3)
F(10)	0.078(3)	0.377(16)	0.076(3)	0.021(6)	0.014(3)	-0.029(6)
F(11)	0.085(3)	0.176(6)	0.087(3)	0.008(4)	0.037(3)	-0.017(4)
F(12)	0.258(11)	0.108(5)	0.160(7)	-0.052(5)	0.114(8)	-0.055(6)
P(5)	0.128(2)	0.142(3)	0.0991(19)	-0.0070(19)	0.0273(17)	0.036(2)
F(13)	0.329(19)	0.221(14)	0.229(13)	-0.071(11)	0.070(13)	0.129(14)
F(14)	0.168(8)	0.194(10)	0.133(6)	0.005(6)	0.004(6)	0.020(7)
F(15)	0.252(12)	0.115(6)	0.151(7)	0.014(5)	0.038(8)	-0.011(7)
F(16)	0.167(9)	0.224(13)	0.215(11)	0.016(9)	-0.043(8)	0.039(9)
F(17)	0.184(10)	0.38(2)	0.185(9)	0.089(12)	0.110(9)	0.064(12)
F(18)	0.252(12)	0.126(6)	0.206(10)	-0.023(6)	0.113(10)	-0.004(7)
P(6)	0.0511(7)	0.0838(12)	0.0867(12)	0.0077(10)	0.0191(8)	0.0082(8)
F(19)	0.0505(18)	0.081(3)	0.108(3)	0.015(2)	0.0163(19)	0.0073(18)
F(20)	0.134(5)	0.085(4)	0.282(11)	0.011(5)	-0.105(7)	-0.026(4)
F(21)	0.101(4)	0.166(6)	0.119(4)	0.049(4)	0.059(3)	0.063(4)
F(22)	0.107(4)	0.088(4)	0.167(6)	0.009(4)	-0.016(4)	-0.008(3)
F(23)	0.106(4)	0.181(7)	0.106(4)	0.030(4)	0.046(3)	0.051(4)
F(24)	0.077(3)	0.118(4)	0.097(3)	0.026(3)	0.024(2)	0.027(3)
O(1)	0.119(9)	0.065(6)	0.089(8)	-0.006(6)	-0.008(7)	0.024(6)
O(2)	0.172(16)	0.086(9)	0.143(14)	-0.047(9)	-0.044(12)	0.040(10)
O(3)	0.131(14)	0.134(15)	0.22(2)	-0.015(15)	0.079(15)	-0.029(12)

Table 4. Bond lengths [Å] for ckjsm2302.

atom-atom	distance	atom-atom	distance
P(1)-C(6)	1.758(11)	P(1)-C(12)	1.760(11)
P(1)-C(18)	1.775(9)	P(1)-C(1)	1.802(9)
P(1)-C(12A)	1.856(13)	N(1)-C(5)	1.320(9)
N(1)-C(24)	1.440(10)	N(1)-C(3)	1.498(9)
N(2)-C(5)	1.305(10)	N(2)-C(33)	1.443(10)
N(2)-C(4)	1.485(9)	C(1)-C(2)	1.533(11)
C(1)-H(1A)	0.9900	C(1)-H(1B)	0.9900
C(2)-C(3)	1.551(10)	C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900	C(3)-C(4)	1.533(12)
C(3)-H(3)	1.0000	C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900	C(5)-H(5)	0.9500
C(6)-C(7)	1.409(13)	C(6)-C(11)	1.410(13)
C(7)-C(8)	1.365(15)	C(7)-H(7)	0.9500
C(8)-C(9)	1.364(14)	C(8)-H(8)	0.9500
C(9)-C(10)	1.387(16)	C(9)-H(9)	0.9500
C(10)-C(11)	1.374(17)	C(10)-H(10)	0.9500
C(11)-H(11)	0.9500	C(12)-C(13)	1.3900
C(12)-C(17)	1.3900	C(13)-C(14)	1.3900
C(13)-H(13)	0.9500	C(14)-C(15)	1.3900
C(14)-H(14)	0.9500	C(15)-C(16)	1.3900
C(15)-H(15)	0.9500	C(16)-C(17)	1.3900
C(16)-H(16)	0.9500	C(17)-H(17)	0.9500
C(12A)-C(13A)	1.3900	C(12A)-C(17A)	1.3900
C(13A)-C(14A)	1.3900	C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.3900	C(14A)-H(14A)	0.9500
C(15A)-C(16A)	1.3900	C(15A)-H(15A)	0.9500
C(16A)-C(17A)	1.3900	C(16A)-H(16A)	0.9500
C(17A)-H(17A)	0.9500	C(18)-C(23)	1.401(12)
C(18)-C(19)	1.432(14)	C(19)-C(20)	1.367(14)
C(19)-H(19)	0.9500	C(20)-C(21)	1.376(14)
C(20)-H(20)	0.9500	C(21)-C(22)	1.408(13)
C(21)-H(21)	0.9500	C(22)-C(23)	1.402(12)
C(22)-H(22)	0.9500	C(23)-H(23)	0.9500
C(24)-C(25)	1.399(10)	C(24)-C(29)	1.408(10)
C(25)-C(26)	1.379(13)	C(25)-C(30)	1.500(12)
C(26)-C(27)	1.378(14)	C(26)-H(26)	0.9500
C(27)-C(28)	1.392(14)	C(27)-C(31)	1.527(14)
C(28)-C(29)	1.371(13)	C(28)-H(28)	0.9500
C(29)-C(32)	1.487(12)	C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800	C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800	C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800	C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800	C(32)-H(32C)	0.9800
C(33)-C(34)	1.392(10)	C(33)-C(38)	1.398(11)
C(34)-C(35)	1.386(11)	C(34)-C(39)	1.515(11)
C(35)-C(36)	1.383(12)	C(35)-H(35)	0.9500
C(36)-C(37)	1.383(11)	C(36)-C(40)	1.548(12)

C(37)-C(38)	1.383(12)	C(37)-H(37)	0.9500
C(38)-C(41)	1.518(11)	C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800	C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800	C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800	C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800	C(41)-H(41C)	0.9800
P(2)-C(47)	1.615(11)	P(2)-C(59)	1.754(13)
P(2)-C(53)	1.770(10)	P(2)-C(42)	1.834(15)
C(42)-C(43)	1.55(2)	C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900	C(43)-C(44)	1.657(17)
C(43)-H(43A)	0.9900	C(43)-H(43B)	0.9900
P(2A)-C(59A)	1.766(13)	P(2A)-C(53)	1.862(11)
P(2A)-C(47)	1.984(13)	P(2A)-C(42A)	2.18(2)
C(43A)-C(42A)	1.50(3)	C(43A)-C(44)	1.509(18)
C(43A)-H(43C)	0.9900	C(43A)-H(43D)	0.9900
C(42A)-H(42C)	0.9900	C(42A)-H(42D)	0.9900
N(3)-C(46)	1.312(10)	N(3)-C(44)	1.475(12)
N(3)-C(65)	1.476(13)	N(4)-C(46)	1.296(11)
N(4)-C(74)	1.430(11)	N(4)-C(45)	1.474(9)
C(44)-C(45)	1.551(17)	C(44)-H(44)	1.0000
C(44)-H(44A)	1.0000	C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900	C(46)-H(46)	0.9500
C(47)-C(48)	1.380(16)	C(47)-C(52)	1.393(12)
C(48)-C(49)	1.38(2)	C(48)-H(48)	0.9500
C(49)-C(50)	1.41(2)	C(49)-H(49)	0.9500
C(50)-C(51)	1.366(16)	C(50)-H(50)	0.9500
C(51)-C(52)	1.392(13)	C(51)-H(51)	0.9500
C(52)-H(52)	0.9500	C(53)-C(54)	1.391(15)
C(53)-C(58)	1.401(13)	C(54)-C(55)	1.409(14)
C(54)-H(54)	0.9500	C(55)-C(56)	1.375(14)
C(55)-H(55)	0.9500	C(56)-C(57)	1.380(15)
C(56)-H(56)	0.9500	C(57)-C(58)	1.396(13)
C(57)-H(57)	0.9500	C(58)-H(58)	0.9500
C(59)-C(60)	1.3900	C(59)-C(64)	1.3900
C(60)-C(61)	1.3900	C(60)-H(60)	0.9500
C(61)-C(62)	1.3900	C(61)-H(61)	0.9500
C(62)-C(63)	1.3900	C(62)-H(62)	0.9500
C(63)-C(64)	1.3900	C(63)-H(63)	0.9500
C(64)-H(64)	0.9500	C(63A)-C(62A)	1.3900
C(63A)-C(64A)	1.3900	C(63A)-H(63A)	0.9500
C(62A)-C(61A)	1.3900	C(62A)-H(62A)	0.9500
C(61A)-C(60A)	1.3900	C(61A)-H(61A)	0.9500
C(60A)-C(59A)	1.3900	C(60A)-H(60A)	0.9500
C(59A)-C(64A)	1.3900	C(64A)-H(64A)	0.9500
C(65)-C(70)	1.367(12)	C(65)-C(66)	1.379(14)
C(66)-C(67)	1.380(16)	C(66)-C(71)	1.511(12)
C(67)-C(68)	1.403(13)	C(67)-H(67)	0.9500
C(68)-C(69)	1.376(17)	C(68)-C(72)	1.502(18)
C(69)-C(70)	1.424(19)	C(69)-H(69)	0.9500
C(70)-C(73)	1.523(17)	C(71)-H(71A)	0.9800
C(71)-H(71B)	0.9800	C(71)-H(71C)	0.9800

C(72)-H(72A)	0.9800	C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800	C(73)-H(73A)	0.9800
C(73)-H(73B)	0.9800	C(73)-H(73C)	0.9800
C(74)-C(75)	1.393(15)	C(74)-C(79)	1.399(13)
C(75)-C(76)	1.423(15)	C(75)-C(80)	1.512(14)
C(76)-C(77)	1.350(17)	C(76)-H(76)	0.9500
C(77)-C(78)	1.435(19)	C(77)-C(81)	1.519(15)
C(78)-C(79)	1.404(15)	C(78)-H(78)	0.9500
C(79)-C(82)	1.511(16)	C(80)-H(80A)	0.9800
C(80)-H(80B)	0.9800	C(80)-H(80C)	0.9800
C(81)-H(81A)	0.9800	C(81)-H(81B)	0.9800
C(81)-H(81C)	0.9800	C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800	C(82)-H(82C)	0.9800
P(3)-F(4)	1.515(13)	P(3)-F(2)	1.525(10)
P(3)-F(6)	1.564(7)	P(3)-F(1)	1.569(8)
P(3)-F(3)	1.621(9)	P(3)-F(5)	1.628(10)
P(4)-F(12)	1.560(8)	P(4)-F(10)	1.571(7)
P(4)-F(11)	1.580(5)	P(4)-F(8)	1.589(6)
P(4)-F(9)	1.594(5)	P(4)-F(7)	1.601(7)
P(5)-F(13)	1.538(11)	P(5)-F(16)	1.548(12)
P(5)-F(15)	1.549(11)	P(5)-F(17)	1.553(13)
P(5)-F(18)	1.562(11)	P(5)-F(14)	1.586(10)
P(6)-F(20)	1.521(6)	P(6)-F(21)	1.570(6)
P(6)-F(23)	1.571(6)	P(6)-F(24)	1.591(5)
P(6)-F(19)	1.599(5)	P(6)-F(22)	1.619(7)
O(1)-H(1OA)	0.8499	O(1)-H(1OB)	0.8500
O(2)-H(2OA)	0.8501	O(2)-H(2OB)	0.8498
O(3)-H(3OA)	0.8501	O(3)-H(3OB)	0.8500

Symmetry transformations used to generate equivalent atoms:

Table 5. Bond angles [°] for ckjsm2302.

atom-atom-atom	angle	atom-atom-atom	angle
C(6)-P(1)-C(12)	101.2(6)	C(6)-P(1)-C(18)	111.9(4)
C(12)-P(1)-C(18)	113.8(7)	C(6)-P(1)-C(1)	111.2(4)
C(12)-P(1)-C(1)	110.1(6)	C(18)-P(1)-C(1)	108.5(4)
C(6)-P(1)-C(12A)	116.9(6)	C(18)-P(1)-C(12A)	104.2(7)
C(1)-P(1)-C(12A)	103.6(7)	C(5)-N(1)-C(24)	126.3(6)
C(5)-N(1)-C(3)	109.6(6)	C(24)-N(1)-C(3)	124.0(6)
C(5)-N(2)-C(33)	126.4(6)	C(5)-N(2)-C(4)	110.2(6)
C(33)-N(2)-C(4)	123.4(6)	C(2)-C(1)-P(1)	114.9(6)
C(2)-C(1)-H(1A)	108.6	P(1)-C(1)-H(1A)	108.6
C(2)-C(1)-H(1B)	108.6	P(1)-C(1)-H(1B)	108.6
H(1A)-C(1)-H(1B)	107.5	C(1)-C(2)-C(3)	110.9(6)
C(1)-C(2)-H(2A)	109.5	C(3)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5	C(3)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	108.1	N(1)-C(3)-C(4)	102.1(5)
N(1)-C(3)-C(2)	113.6(6)	C(4)-C(3)-C(2)	113.6(6)
N(1)-C(3)-H(3)	109.1	C(4)-C(3)-H(3)	109.1
C(2)-C(3)-H(3)	109.1	N(2)-C(4)-C(3)	103.0(6)
N(2)-C(4)-H(4A)	111.2	C(3)-C(4)-H(4A)	111.2
N(2)-C(4)-H(4B)	111.2	C(3)-C(4)-H(4B)	111.2
H(4A)-C(4)-H(4B)	109.1	N(2)-C(5)-N(1)	113.8(6)
N(2)-C(5)-H(5)	123.1	N(1)-C(5)-H(5)	123.1
C(7)-C(6)-C(11)	117.0(10)	C(7)-C(6)-P(1)	121.1(7)
C(11)-C(6)-P(1)	121.6(8)	C(8)-C(7)-C(6)	120.5(8)
C(8)-C(7)-H(7)	119.8	C(6)-C(7)-H(7)	119.8
C(9)-C(8)-C(7)	121.9(10)	C(9)-C(8)-H(8)	119.1
C(7)-C(8)-H(8)	119.1	C(8)-C(9)-C(10)	119.4(12)
C(8)-C(9)-H(9)	120.3	C(10)-C(9)-H(9)	120.3
C(11)-C(10)-C(9)	120.0(10)	C(11)-C(10)-H(10)	120.0
C(9)-C(10)-H(10)	120.0	C(10)-C(11)-C(6)	121.3(10)
C(10)-C(11)-H(11)	119.3	C(6)-C(11)-H(11)	119.3
C(13)-C(12)-C(17)	120.0	C(13)-C(12)-P(1)	120.3(8)
C(17)-C(12)-P(1)	118.8(8)	C(14)-C(13)-C(12)	120.0
C(14)-C(13)-H(13)	120.0	C(12)-C(13)-H(13)	120.0
C(13)-C(14)-C(15)	120.0	C(13)-C(14)-H(14)	120.0
C(15)-C(14)-H(14)	120.0	C(16)-C(15)-C(14)	120.0
C(16)-C(15)-H(15)	120.0	C(14)-C(15)-H(15)	120.0
C(17)-C(16)-C(15)	120.0	C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0	C(16)-C(17)-C(12)	120.0
C(16)-C(17)-H(17)	120.0	C(12)-C(17)-H(17)	120.0
C(13A)-C(12A)-C(17A)	120.0	C(13A)-C(12A)-P(1)	116.0(10)
C(17A)-C(12A)-P(1)	123.8(10)	C(12A)-C(13A)-C(14A)	120.0
C(12A)-C(13A)-H(13A)	120.0	C(14A)-C(13A)-H(13A)	120.0
C(13A)-C(14A)-C(15A)	120.0	C(13A)-C(14A)-H(14A)	120.0
C(15A)-C(14A)-H(14A)	120.0	C(16A)-C(15A)-C(14A)	120.0
C(16A)-C(15A)-H(15A)	120.0	C(14A)-C(15A)-H(15A)	120.0
C(15A)-C(16A)-C(17A)	120.0	C(15A)-C(16A)-H(16A)	120.0
C(17A)-C(16A)-H(16A)	120.0	C(16A)-C(17A)-C(12A)	120.0

C(16A)-C(17A)-H(17A)	120.0	C(12A)-C(17A)-H(17A)	120.0
C(23)-C(18)-C(19)	119.4(8)	C(23)-C(18)-P(1)	118.8(7)
C(19)-C(18)-P(1)	121.7(7)	C(20)-C(19)-C(18)	118.9(9)
C(20)-C(19)-H(19)	120.5	C(18)-C(19)-H(19)	120.5
C(19)-C(20)-C(21)	122.5(10)	C(19)-C(20)-H(20)	118.7
C(21)-C(20)-H(20)	118.7	C(20)-C(21)-C(22)	119.5(8)
C(20)-C(21)-H(21)	120.3	C(22)-C(21)-H(21)	120.3
C(23)-C(22)-C(21)	119.7(8)	C(23)-C(22)-H(22)	120.1
C(21)-C(22)-H(22)	120.1	C(18)-C(23)-C(22)	120.0(9)
C(18)-C(23)-H(23)	120.0	C(22)-C(23)-H(23)	120.0
C(25)-C(24)-C(29)	122.8(7)	C(25)-C(24)-N(1)	118.6(7)
C(29)-C(24)-N(1)	118.6(6)	C(26)-C(25)-C(24)	117.0(8)
C(26)-C(25)-C(30)	120.9(8)	C(24)-C(25)-C(30)	122.1(8)
C(27)-C(26)-C(25)	123.3(8)	C(27)-C(26)-H(26)	118.4
C(25)-C(26)-H(26)	118.4	C(26)-C(27)-C(28)	116.7(9)
C(26)-C(27)-C(31)	120.9(9)	C(28)-C(27)-C(31)	122.4(9)
C(29)-C(28)-C(27)	124.4(8)	C(29)-C(28)-H(28)	117.8
C(27)-C(28)-H(28)	117.8	C(28)-C(29)-C(24)	115.7(8)
C(28)-C(29)-C(32)	121.6(8)	C(24)-C(29)-C(32)	122.7(8)
C(25)-C(30)-H(30A)	109.5	C(25)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5	C(25)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5	H(30B)-C(30)-H(30C)	109.5
C(27)-C(31)-H(31A)	109.5	C(27)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5	C(27)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5	H(31B)-C(31)-H(31C)	109.5
C(29)-C(32)-H(32A)	109.5	C(29)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5	C(29)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5	H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-C(38)	122.5(7)	C(34)-C(33)-N(2)	119.2(7)
C(38)-C(33)-N(2)	118.3(6)	C(35)-C(34)-C(33)	118.4(7)
C(35)-C(34)-C(39)	120.6(7)	C(33)-C(34)-C(39)	121.0(7)
C(36)-C(35)-C(34)	119.8(7)	C(36)-C(35)-H(35)	120.1
C(34)-C(35)-H(35)	120.1	C(35)-C(36)-C(37)	121.0(8)
C(35)-C(36)-C(40)	118.7(8)	C(37)-C(36)-C(40)	120.3(8)
C(38)-C(37)-C(36)	120.8(8)	C(38)-C(37)-H(37)	119.6
C(36)-C(37)-H(37)	119.6	C(37)-C(38)-C(33)	117.4(7)
C(37)-C(38)-C(41)	121.4(7)	C(33)-C(38)-C(41)	121.2(7)
C(34)-C(39)-H(39A)	109.5	C(34)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5	C(34)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5	H(39B)-C(39)-H(39C)	109.5
C(36)-C(40)-H(40A)	109.5	C(36)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5	C(36)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5	H(40B)-C(40)-H(40C)	109.5
C(38)-C(41)-H(41A)	109.5	C(38)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5	C(38)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5	H(41B)-C(41)-H(41C)	109.5
C(47)-P(2)-C(59)	101.2(6)	C(47)-P(2)-C(53)	118.2(6)
C(59)-P(2)-C(53)	105.1(7)	C(47)-P(2)-C(42)	129.9(7)
C(59)-P(2)-C(42)	81.0(8)	C(53)-P(2)-C(42)	108.9(6)
C(43)-C(42)-P(2)	99.8(11)	C(43)-C(42)-H(42A)	111.8
P(2)-C(42)-H(42A)	111.8	C(43)-C(42)-H(42B)	111.8

P(2)-C(42)-H(42B)	111.8	H(42A)-C(42)-H(42B)	109.5
C(42)-C(43)-C(44)	103.4(11)	C(42)-C(43)-H(43A)	111.1
C(44)-C(43)-H(43A)	111.1	C(42)-C(43)-H(43B)	111.1
C(44)-C(43)-H(43B)	111.1	H(43A)-C(43)-H(43B)	109.0
C(59A)-P(2A)-C(53)	121.2(7)	C(59A)-P(2A)-C(47)	111.3(7)
C(53)-P(2A)-C(47)	98.1(5)	C(59A)-P(2A)-C(42A)	137.4(8)
C(53)-P(2A)-C(42A)	93.3(6)	C(47)-P(2A)-C(42A)	84.8(6)
C(42A)-C(43A)-C(44)	105.0(15)	C(42A)-C(43A)-H(43C)	110.7
C(44)-C(43A)-H(43C)	110.7	C(42A)-C(43A)-H(43D)	110.7
C(44)-C(43A)-H(43D)	110.7	H(43C)-C(43A)-H(43D)	108.8
C(43A)-C(42A)-P(2A)	98.5(15)	C(43A)-C(42A)-H(42C)	112.1
P(2A)-C(42A)-H(42C)	112.1	C(43A)-C(42A)-H(42D)	112.1
P(2A)-C(42A)-H(42D)	112.1	H(42C)-C(42A)-H(42D)	109.7
C(46)-N(3)-C(44)	110.3(8)	C(46)-N(3)-C(65)	121.4(7)
C(44)-N(3)-C(65)	126.0(7)	C(46)-N(4)-C(74)	124.3(6)
C(46)-N(4)-C(45)	109.0(8)	C(74)-N(4)-C(45)	126.7(8)
N(3)-C(44)-C(43A)	127.6(12)	N(3)-C(44)-C(45)	100.5(6)
C(43A)-C(44)-C(45)	97.6(11)	N(3)-C(44)-C(43)	100.8(9)
C(45)-C(44)-C(43)	124.8(10)	N(3)-C(44)-H(44)	109.7
C(45)-C(44)-H(44)	109.7	C(43)-C(44)-H(44)	109.7
N(3)-C(44)-H(44A)	109.6	C(43A)-C(44)-H(44A)	109.6
C(45)-C(44)-H(44A)	109.6	N(4)-C(45)-C(44)	103.5(8)
N(4)-C(45)-H(45A)	111.1	C(44)-C(45)-H(45A)	111.1
N(4)-C(45)-H(45B)	111.1	C(44)-C(45)-H(45B)	111.1
H(45A)-C(45)-H(45B)	109.0	N(4)-C(46)-N(3)	114.4(7)
N(4)-C(46)-H(46)	122.8	N(3)-C(46)-H(46)	122.8
C(48)-C(47)-C(52)	119.9(11)	C(48)-C(47)-P(2)	115.1(8)
C(52)-C(47)-P(2)	124.3(9)	C(48)-C(47)-P(2A)	128.3(9)
C(52)-C(47)-P(2A)	111.7(8)	C(47)-C(48)-C(49)	121.9(12)
C(47)-C(48)-H(48)	119.0	C(49)-C(48)-H(48)	119.0
C(48)-C(49)-C(50)	117.4(12)	C(48)-C(49)-H(49)	121.3
C(50)-C(49)-H(49)	121.3	C(51)-C(50)-C(49)	121.2(12)
C(51)-C(50)-H(50)	119.4	C(49)-C(50)-H(50)	119.4
C(50)-C(51)-C(52)	120.8(11)	C(50)-C(51)-H(51)	119.6
C(52)-C(51)-H(51)	119.6	C(51)-C(52)-C(47)	118.8(10)
C(51)-C(52)-H(52)	120.6	C(47)-C(52)-H(52)	120.6
C(54)-C(53)-C(58)	120.5(8)	C(54)-C(53)-P(2)	112.4(7)
C(58)-C(53)-P(2)	126.1(8)	C(54)-C(53)-P(2A)	129.1(7)
C(58)-C(53)-P(2A)	110.3(8)	C(53)-C(54)-C(55)	118.4(9)
C(53)-C(54)-H(54)	120.8	C(55)-C(54)-H(54)	120.8
C(56)-C(55)-C(54)	120.9(10)	C(56)-C(55)-H(55)	119.6
C(54)-C(55)-H(55)	119.6	C(55)-C(56)-C(57)	120.5(8)
C(55)-C(56)-H(56)	119.7	C(57)-C(56)-H(56)	119.7
C(56)-C(57)-C(58)	119.9(9)	C(56)-C(57)-H(57)	120.1
C(58)-C(57)-H(57)	120.1	C(57)-C(58)-C(53)	119.7(10)
C(57)-C(58)-H(58)	120.2	C(53)-C(58)-H(58)	120.2
C(60)-C(59)-C(64)	120.0	C(60)-C(59)-P(2)	121.0(8)
C(64)-C(59)-P(2)	118.5(8)	C(59)-C(60)-C(61)	120.0
C(59)-C(60)-H(60)	120.0	C(61)-C(60)-H(60)	120.0
C(62)-C(61)-C(60)	120.0	C(62)-C(61)-H(61)	120.0
C(60)-C(61)-H(61)	120.0	C(61)-C(62)-C(63)	120.0

C(61)-C(62)-H(62)	120.0	C(63)-C(62)-H(62)	120.0
C(62)-C(63)-C(64)	120.0	C(62)-C(63)-H(63)	120.0
C(64)-C(63)-H(63)	120.0	C(63)-C(64)-C(59)	120.0
C(63)-C(64)-H(64)	120.0	C(59)-C(64)-H(64)	120.0
C(62A)-C(63A)-C(64A)	120.0	C(62A)-C(63A)-H(63A)	120.0
C(64A)-C(63A)-H(63A)	120.0	C(63A)-C(62A)-C(61A)	120.0
C(63A)-C(62A)-H(62A)	120.0	C(61A)-C(62A)-H(62A)	120.0
C(60A)-C(61A)-C(62A)	120.0	C(60A)-C(61A)-H(61A)	120.0
C(62A)-C(61A)-H(61A)	120.0	C(61A)-C(60A)-C(59A)	120.0
C(61A)-C(60A)-H(60A)	120.0	C(59A)-C(60A)-H(60A)	120.0
C(64A)-C(59A)-C(60A)	120.0	C(64A)-C(59A)-P(2A)	118.0(9)
C(60A)-C(59A)-P(2A)	121.9(9)	C(59A)-C(64A)-C(63A)	120.0
C(59A)-C(64A)-H(64A)	120.0	C(63A)-C(64A)-H(64A)	120.0
C(70)-C(65)-C(66)	123.9(11)	C(70)-C(65)-N(3)	117.8(10)
C(66)-C(65)-N(3)	118.3(8)	C(65)-C(66)-C(67)	117.7(8)
C(65)-C(66)-C(71)	122.5(11)	C(67)-C(66)-C(71)	119.7(10)
C(66)-C(67)-C(68)	121.9(11)	C(66)-C(67)-H(67)	119.1
C(68)-C(67)-H(67)	119.1	C(69)-C(68)-C(67)	118.0(11)
C(69)-C(68)-C(72)	121.8(10)	C(67)-C(68)-C(72)	120.0(11)
C(68)-C(69)-C(70)	121.8(9)	C(68)-C(69)-H(69)	119.1
C(70)-C(69)-H(69)	119.1	C(65)-C(70)-C(69)	116.7(11)
C(65)-C(70)-C(73)	124.2(12)	C(69)-C(70)-C(73)	119.2(9)
C(66)-C(71)-H(71A)	109.5	C(66)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5	C(66)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5	H(71B)-C(71)-H(71C)	109.5
C(68)-C(72)-H(72A)	109.5	C(68)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5	C(68)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5	H(72B)-C(72)-H(72C)	109.5
C(70)-C(73)-H(73A)	109.5	C(70)-C(73)-H(73B)	109.5
H(73A)-C(73)-H(73B)	109.5	C(70)-C(73)-H(73C)	109.5
H(73A)-C(73)-H(73C)	109.5	H(73B)-C(73)-H(73C)	109.5
C(75)-C(74)-C(79)	122.9(8)	C(75)-C(74)-N(4)	117.2(8)
C(79)-C(74)-N(4)	119.7(9)	C(74)-C(75)-C(76)	118.1(10)
C(74)-C(75)-C(80)	121.1(9)	C(76)-C(75)-C(80)	120.7(11)
C(77)-C(76)-C(75)	121.3(12)	C(77)-C(76)-H(76)	119.4
C(75)-C(76)-H(76)	119.4	C(76)-C(77)-C(78)	119.4(10)
C(76)-C(77)-C(81)	120.8(13)	C(78)-C(77)-C(81)	119.8(11)
C(79)-C(78)-C(77)	121.2(10)	C(79)-C(78)-H(78)	119.4
C(77)-C(78)-H(78)	119.4	C(74)-C(79)-C(78)	117.0(10)
C(74)-C(79)-C(82)	121.8(8)	C(78)-C(79)-C(82)	121.2(9)
C(75)-C(80)-H(80A)	109.5	C(75)-C(80)-H(80B)	109.5
H(80A)-C(80)-H(80B)	109.5	C(75)-C(80)-H(80C)	109.5
H(80A)-C(80)-H(80C)	109.5	H(80B)-C(80)-H(80C)	109.5
C(77)-C(81)-H(81A)	109.5	C(77)-C(81)-H(81B)	109.5
H(81A)-C(81)-H(81B)	109.5	C(77)-C(81)-H(81C)	109.5
H(81A)-C(81)-H(81C)	109.5	H(81B)-C(81)-H(81C)	109.5
C(79)-C(82)-H(82A)	109.5	C(79)-C(82)-H(82B)	109.5
H(82A)-C(82)-H(82B)	109.5	C(79)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5	H(82B)-C(82)-H(82C)	109.5
F(4)-P(3)-F(2)	176.7(7)	F(4)-P(3)-F(6)	92.4(6)
F(2)-P(3)-F(6)	90.8(6)	F(4)-P(3)-F(1)	87.4(9)

F(2)-P(3)-F(1)	89.4(8)	F(6)-P(3)-F(1)	178.9(7)
F(4)-P(3)-F(3)	92.1(7)	F(2)-P(3)-F(3)	87.9(4)
F(6)-P(3)-F(3)	90.7(5)	F(1)-P(3)-F(3)	88.2(5)
F(4)-P(3)-F(5)	90.7(6)	F(2)-P(3)-F(5)	89.2(5)
F(6)-P(3)-F(5)	91.6(5)	F(1)-P(3)-F(5)	89.5(5)
F(3)-P(3)-F(5)	176.3(4)	F(12)-P(4)-F(10)	92.5(7)
F(12)-P(4)-F(11)	90.7(5)	F(10)-P(4)-F(11)	89.9(3)
F(12)-P(4)-F(8)	89.7(5)	F(10)-P(4)-F(8)	177.5(6)
F(11)-P(4)-F(8)	88.9(3)	F(12)-P(4)-F(9)	90.1(4)
F(10)-P(4)-F(9)	89.9(3)	F(11)-P(4)-F(9)	179.1(4)
F(8)-P(4)-F(9)	91.3(3)	F(12)-P(4)-F(7)	177.2(6)
F(10)-P(4)-F(7)	89.9(6)	F(11)-P(4)-F(7)	90.8(4)
F(8)-P(4)-F(7)	88.0(4)	F(9)-P(4)-F(7)	88.4(4)
F(13)-P(5)-F(16)	95.2(9)	F(13)-P(5)-F(15)	89.5(9)
F(16)-P(5)-F(15)	95.0(7)	F(13)-P(5)-F(17)	93.5(10)
F(16)-P(5)-F(17)	87.5(8)	F(15)-P(5)-F(17)	175.9(7)
F(13)-P(5)-F(18)	175.6(10)	F(16)-P(5)-F(18)	87.6(8)
F(15)-P(5)-F(18)	86.8(6)	F(17)-P(5)-F(18)	90.0(8)
F(13)-P(5)-F(14)	90.8(8)	F(16)-P(5)-F(14)	172.8(8)
F(15)-P(5)-F(14)	89.1(6)	F(17)-P(5)-F(14)	88.1(7)
F(18)-P(5)-F(14)	86.7(7)	F(20)-P(6)-F(21)	91.3(6)
F(20)-P(6)-F(23)	96.7(6)	F(21)-P(6)-F(23)	172.0(5)
F(20)-P(6)-F(24)	91.4(4)	F(21)-P(6)-F(24)	90.0(3)
F(23)-P(6)-F(24)	90.3(3)	F(20)-P(6)-F(19)	89.7(3)
F(21)-P(6)-F(19)	90.8(3)	F(23)-P(6)-F(19)	88.8(3)
F(24)-P(6)-F(19)	178.7(3)	F(20)-P(6)-F(22)	176.5(6)
F(21)-P(6)-F(22)	85.4(5)	F(23)-P(6)-F(22)	86.6(5)
F(24)-P(6)-F(22)	89.6(4)	F(19)-P(6)-F(22)	89.4(3)
H(1OA)-O(1)-H(1OB)	110.5	H(2OA)-O(2)-H(2OB)	104.5
H(3OA)-O(3)-H(3OB)	104.4		

Symmetry transformations used to generate equivalent atoms:

Table 6. Torsion angles [°] for ckjsm2302.

atom-atom-atom-atom	angle	atom-atom-atom-atom	angle
C(6)-P(1)-C(1)-C(2)	56.2(7)	C(12)-P(1)-C(1)-C(2)	167.6(8)
C(18)-P(1)-C(1)-C(2)	-67.3(8)	C(12A)-P(1)-C(1)-C(2)	-177.5(8)
P(1)-C(1)-C(2)-C(3)	174.8(6)	C(5)-N(1)-C(3)-C(4)	-10.6(7)
C(24)-N(1)-C(3)-C(4)	173.2(6)	C(5)-N(1)-C(3)-C(2)	-133.4(6)
C(24)-N(1)-C(3)-C(2)	50.4(9)	C(1)-C(2)-C(3)-N(1)	-81.5(8)
C(1)-C(2)-C(3)-C(4)	162.4(7)	C(5)-N(2)-C(4)-C(3)	-8.7(8)
C(33)-N(2)-C(4)-C(3)	171.7(6)	N(1)-C(3)-C(4)-N(2)	11.0(7)
C(2)-C(3)-C(4)-N(2)	133.8(6)	C(33)-N(2)-C(5)-N(1)	-178.3(6)
C(4)-N(2)-C(5)-N(1)	2.2(9)	C(24)-N(1)-C(5)-N(2)	-178.1(6)
C(3)-N(1)-C(5)-N(2)	5.8(8)	C(12)-P(1)-C(6)-C(7)	-82.6(9)
C(18)-P(1)-C(6)-C(7)	155.9(6)	C(1)-P(1)-C(6)-C(7)	34.4(7)
C(12A)-P(1)-C(6)-C(7)	-84.2(10)	C(12)-P(1)-C(6)-C(11)	90.4(9)
C(18)-P(1)-C(6)-C(11)	-31.1(8)	C(1)-P(1)-C(6)-C(11)	-152.7(7)
C(12A)-P(1)-C(6)-C(11)	88.8(10)	C(11)-C(6)-C(7)-C(8)	-0.3(12)
P(1)-C(6)-C(7)-C(8)	173.0(7)	C(6)-C(7)-C(8)-C(9)	0.1(14)
C(7)-C(8)-C(9)-C(10)	0.8(15)	C(8)-C(9)-C(10)-C(11)	-1.4(16)
C(9)-C(10)-C(11)-C(6)	1.2(17)	C(7)-C(6)-C(11)-C(10)	-0.4(14)
P(1)-C(6)-C(11)-C(10)	-173.6(8)	C(6)-P(1)-C(12)-C(13)	-53.4(9)
C(18)-P(1)-C(12)-C(13)	66.7(10)	C(1)-P(1)-C(12)-C(13)	-171.2(8)
C(6)-P(1)-C(12)-C(17)	137.2(9)	C(18)-P(1)-C(12)-C(17)	-102.6(10)
C(1)-P(1)-C(12)-C(17)	19.5(11)	C(17)-C(12)-C(13)-C(14)	0.0
P(1)-C(12)-C(13)-C(14)	-169.2(12)	C(12)-C(13)-C(14)-C(15)	0.0
C(13)-C(14)-C(15)-C(16)	0.0	C(14)-C(15)-C(16)-C(17)	0.0
C(15)-C(16)-C(17)-C(12)	0.0	C(13)-C(12)-C(17)-C(16)	0.0
P(1)-C(12)-C(17)-C(16)	169.4(12)	C(6)-P(1)-C(12A)-C(13A)	-20.7(11)
C(18)-P(1)-C(12A)-C(13A)	103.2(9)	C(1)-P(1)-C(12A)-C(13A)	-143.3(8)
C(6)-P(1)-C(12A)-C(17A)	153.8(10)	C(18)-P(1)-C(12A)-C(17A)	-82.2(12)
C(1)-P(1)-C(12A)-C(17A)	31.2(13)	C(17A)-C(12A)-C(13A)-C(14A)	0.0
P(1)-C(12A)-C(13A)-C(14A)	174.8(14)	C(12A)-C(13A)-C(14A)-C(15A)	0.0
C(13A)-C(14A)-C(15A)-C(16A)	0.0	C(14A)-C(15A)-C(16A)-C(17A)	0.0
C(15A)-C(16A)-C(17A)-C(12A)	0.0	C(13A)-C(12A)-C(17A)-C(16A)	0.0
P(1)-C(12A)-C(17A)-C(16A)	-174.3(15)	C(6)-P(1)-C(18)-C(23)	-42.5(8)
C(12)-P(1)-C(18)-C(23)	-156.4(8)	C(1)-P(1)-C(18)-C(23)	80.6(8)
C(12A)-P(1)-C(18)-C(23)	-169.6(9)	C(6)-P(1)-C(18)-C(19)	141.7(7)
C(12)-P(1)-C(18)-C(19)	27.7(10)	C(1)-P(1)-C(18)-C(19)	-95.3(8)
C(12A)-P(1)-C(18)-C(19)	14.6(11)	C(23)-C(18)-C(19)-C(20)	-0.7(14)
P(1)-C(18)-C(19)-C(20)	175.2(7)	C(18)-C(19)-C(20)-C(21)	0.3(14)
C(19)-C(20)-C(21)-C(22)	0.3(14)	C(20)-C(21)-C(22)-C(23)	-0.5(13)
C(19)-C(18)-C(23)-C(22)	0.5(14)	P(1)-C(18)-C(23)-C(22)	-175.5(7)
C(21)-C(22)-C(23)-C(18)	0.1(14)	C(5)-N(1)-C(24)-C(25)	82.0(10)
C(3)-N(1)-C(24)-C(25)	-102.4(8)	C(5)-N(1)-C(24)-C(29)	-100.6(9)
C(3)-N(1)-C(24)-C(29)	74.9(9)	C(29)-C(24)-C(25)-C(26)	-4.7(12)
N(1)-C(24)-C(25)-C(26)	172.6(8)	C(29)-C(24)-C(25)-C(30)	174.4(8)
N(1)-C(24)-C(25)-C(30)	-8.4(12)	C(24)-C(25)-C(26)-C(27)	1.2(15)
C(30)-C(25)-C(26)-C(27)	-177.9(10)	C(25)-C(26)-C(27)-C(28)	1.6(17)
C(25)-C(26)-C(27)-C(31)	-178.2(11)	C(26)-C(27)-C(28)-C(29)	-1.1(17)
C(31)-C(27)-C(28)-C(29)	178.7(11)	C(27)-C(28)-C(29)-C(24)	-2.1(15)

C(27)-C(28)-C(29)-C(32)	177.6(10)	C(25)-C(24)-C(29)-C(28)	5.1(12)
N(1)-C(24)-C(29)-C(28)	-172.2(8)	C(25)-C(24)-C(29)-C(32)	-174.6(8)
N(1)-C(24)-C(29)-C(32)	8.1(11)	C(5)-N(2)-C(33)-C(34)	-92.5(9)
C(4)-N(2)-C(33)-C(34)	87.1(9)	C(5)-N(2)-C(33)-C(38)	89.5(9)
C(4)-N(2)-C(33)-C(38)	-91.0(9)	C(38)-C(33)-C(34)-C(35)	3.2(10)
N(2)-C(33)-C(34)-C(35)	-174.8(6)	C(38)-C(33)-C(34)-C(39)	-176.0(7)
N(2)-C(33)-C(34)-C(39)	6.0(10)	C(33)-C(34)-C(35)-C(36)	-1.3(10)
C(39)-C(34)-C(35)-C(36)	177.9(7)	C(34)-C(35)-C(36)-C(37)	-0.8(11)
C(34)-C(35)-C(36)-C(40)	177.9(7)	C(35)-C(36)-C(37)-C(38)	1.0(12)
C(40)-C(36)-C(37)-C(38)	-177.6(8)	C(36)-C(37)-C(38)-C(33)	0.7(12)
C(36)-C(37)-C(38)-C(41)	179.1(8)	C(34)-C(33)-C(38)-C(37)	-2.9(11)
N(2)-C(33)-C(38)-C(37)	175.1(7)	C(34)-C(33)-C(38)-C(41)	178.8(7)
N(2)-C(33)-C(38)-C(41)	-3.3(11)	C(47)-P(2)-C(42)-C(43)	-106.3(11)
C(59)-P(2)-C(42)-C(43)	156.5(11)	C(53)-P(2)-C(42)-C(43)	53.6(12)
P(2)-C(42)-C(43)-C(44)	165.6(9)	C(44)-C(43A)-C(42A)-P(2A)	-177.9(11)
C(46)-N(3)-C(44)-C(43A)	-122.5(14)	C(65)-N(3)-C(44)-C(43A)	74.7(15)
C(46)-N(3)-C(44)-C(45)	-14.3(9)	C(65)-N(3)-C(44)-C(45)	-177.1(8)
C(46)-N(3)-C(44)-C(43)	-143.1(10)	C(65)-N(3)-C(44)-C(43)	54.2(11)
C(42A)-C(43A)-C(44)-N(3)	-89.3(15)	C(42A)-C(43A)-C(44)-C(45)	161.1(13)
C(42)-C(43)-C(44)-N(3)	-179.6(11)	C(42)-C(43)-C(44)-C(45)	69.4(14)
C(46)-N(4)-C(45)-C(44)	-10.8(10)	C(74)-N(4)-C(45)-C(44)	168.8(8)
N(3)-C(44)-C(45)-N(4)	14.4(9)	C(43A)-C(44)-C(45)-N(4)	145.0(10)
C(43)-C(44)-C(45)-N(4)	125.5(10)	C(74)-N(4)-C(46)-N(3)	-177.7(8)
C(45)-N(4)-C(46)-N(3)	1.9(11)	C(44)-N(3)-C(46)-N(4)	8.7(11)
C(65)-N(3)-C(46)-N(4)	172.4(7)	C(59)-P(2)-C(47)-C(48)	134.5(10)
C(53)-P(2)-C(47)-C(48)	-111.4(10)	C(42)-P(2)-C(47)-C(48)	46.9(15)
C(59)-P(2)-C(47)-C(52)	-55.0(11)	C(53)-P(2)-C(47)-C(52)	59.1(13)
C(42)-P(2)-C(47)-C(52)	-142.6(10)	C(52)-C(47)-C(48)-C(49)	0.5(18)
P(2)-C(47)-C(48)-C(49)	171.4(10)	P(2A)-C(47)-C(48)-C(49)	-176.5(10)
C(47)-C(48)-C(49)-C(50)	0.4(19)	C(48)-C(49)-C(50)-C(51)	-1.6(18)
C(49)-C(50)-C(51)-C(52)	2.0(16)	C(50)-C(51)-C(52)-C(47)	-1.1(14)
C(48)-C(47)-C(52)-C(51)	-0.1(15)	P(2)-C(47)-C(52)-C(51)	-170.2(8)
P(2A)-C(47)-C(52)-C(51)	177.4(7)	C(47)-P(2)-C(53)-C(54)	29.9(11)
C(59)-P(2)-C(53)-C(54)	141.8(9)	C(42)-P(2)-C(53)-C(54)	-132.7(9)
C(47)-P(2)-C(53)-C(58)	-161.5(9)	C(59)-P(2)-C(53)-C(58)	-49.5(11)
C(42)-P(2)-C(53)-C(58)	36.0(13)	C(59A)-P(2A)-C(53)-C(54)	122.6(11)
C(47)-P(2A)-C(53)-C(54)	1.7(11)	C(42A)-P(2A)-C(53)-C(54)	-83.6(11)
C(59A)-P(2A)-C(53)-C(58)	-55.2(10)	C(47)-P(2A)-C(53)-C(58)	-176.1(7)
C(42A)-P(2A)-C(53)-C(58)	98.6(9)	C(58)-C(53)-C(54)-C(55)	-1.0(16)
P(2)-C(53)-C(54)-C(55)	168.4(9)	P(2A)-C(53)-C(54)-C(55)	-178.6(9)
C(53)-C(54)-C(55)-C(56)	-1.7(17)	C(54)-C(55)-C(56)-C(57)	2.8(18)
C(55)-C(56)-C(57)-C(58)	-1.0(18)	C(56)-C(57)-C(58)-C(53)	-1.7(17)
C(54)-C(53)-C(58)-C(57)	2.7(16)	P(2)-C(53)-C(58)-C(57)	-165.1(9)
P(2A)-C(53)-C(58)-C(57)	-179.3(9)	C(47)-P(2)-C(59)-C(60)	93.3(8)
C(53)-P(2)-C(59)-C(60)	-30.3(8)	C(42)-P(2)-C(59)-C(60)	-137.6(8)
C(47)-P(2)-C(59)-C(64)	-78.3(8)	C(53)-P(2)-C(59)-C(64)	158.1(7)
C(42)-P(2)-C(59)-C(64)	50.8(8)	C(64)-C(59)-C(60)-C(61)	0.0
P(2)-C(59)-C(60)-C(61)	-171.4(10)	C(59)-C(60)-C(61)-C(62)	0.0
C(60)-C(61)-C(62)-C(63)	0.0	C(61)-C(62)-C(63)-C(64)	0.0
C(62)-C(63)-C(64)-C(59)	0.0	C(60)-C(59)-C(64)-C(63)	0.0
P(2)-C(59)-C(64)-C(63)	171.6(10)	C(64A)-C(63A)-C(62A)-C(61A)	0.0

C(63A)-C(62A)-C(61A)-C(60A)	0.0	C(62A)-C(61A)-C(60A)-C(59A)	0.0
C(61A)-C(60A)-C(59A)-C(64A)	0.0	C(61A)-C(60A)-C(59A)-P(2A)	-178.2(12)
C(53)-P(2A)-C(59A)-C(64A)	168.3(8)	C(47)-P(2A)-C(59A)-C(64A)	-77.4(10)
C(42A)-P(2A)-C(59A)-C(64A)	28.9(16)	C(53)-P(2A)-C(59A)-C(60A)	-13.5(11)
C(47)-P(2A)-C(59A)-C(60A)	100.8(9)	C(42A)-P(2A)-C(59A)-C(60A)	-152.9(11)
C(60A)-C(59A)-C(64A)-C(63A)	0.0	P(2A)-C(59A)-C(64A)-C(63A)	178.3(11)
C(62A)-C(63A)-C(64A)-C(59A)	0.0	C(46)-N(3)-C(65)-C(70)	94.4(10)
C(44)-N(3)-C(65)-C(70)	-104.6(10)	C(46)-N(3)-C(65)-C(66)	-83.1(9)
C(44)-N(3)-C(65)-C(66)	77.9(10)	C(70)-C(65)-C(66)-C(67)	-0.8(13)
N(3)-C(65)-C(66)-C(67)	176.6(7)	C(70)-C(65)-C(66)-C(71)	-179.3(9)
N(3)-C(65)-C(66)-C(71)	-1.9(11)	C(65)-C(66)-C(67)-C(68)	-1.3(13)
C(71)-C(66)-C(67)-C(68)	177.3(9)	C(66)-C(67)-C(68)-C(69)	1.8(15)
C(66)-C(67)-C(68)-C(72)	-173.8(10)	C(67)-C(68)-C(69)-C(70)	-0.4(16)
C(72)-C(68)-C(69)-C(70)	175.2(11)	C(66)-C(65)-C(70)-C(69)	2.1(14)
N(3)-C(65)-C(70)-C(69)	-175.3(8)	C(66)-C(65)-C(70)-C(73)	-179.8(10)
N(3)-C(65)-C(70)-C(73)	2.8(14)	C(68)-C(69)-C(70)-C(65)	-1.5(16)
C(68)-C(69)-C(70)-C(73)	-179.7(11)	C(46)-N(4)-C(74)-C(75)	91.6(9)
C(45)-N(4)-C(74)-C(75)	-88.0(12)	C(46)-N(4)-C(74)-C(79)	-83.8(12)
C(45)-N(4)-C(74)-C(79)	96.6(10)	C(79)-C(74)-C(75)-C(76)	-0.2(13)
N(4)-C(74)-C(75)-C(76)	-175.5(8)	C(79)-C(74)-C(75)-C(80)	176.1(8)
N(4)-C(74)-C(75)-C(80)	0.8(12)	C(74)-C(75)-C(76)-C(77)	1.6(14)
C(80)-C(75)-C(76)-C(77)	-174.7(9)	C(75)-C(76)-C(77)-C(78)	-2.7(15)
C(75)-C(76)-C(77)-C(81)	178.0(9)	C(76)-C(77)-C(78)-C(79)	2.4(14)
C(81)-C(77)-C(78)-C(79)	-178.2(9)	C(75)-C(74)-C(79)-C(78)	0.0(12)
N(4)-C(74)-C(79)-C(78)	175.1(7)	C(75)-C(74)-C(79)-C(82)	-178.9(8)
N(4)-C(74)-C(79)-C(82)	-3.7(12)	C(77)-C(78)-C(79)-C(74)	-1.1(12)
C(77)-C(78)-C(79)-C(82)	177.8(8)		

Symmetry transformations used to generate equivalent atoms:

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