Electronic Supplementary Material (ESI) for Dalton Transactions.

The Phosphinoboration of Acyl Chlorides

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Supporting Information

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NMR spectra also contain minor amounts of residual solvent peaks. Please see the following paper which lists chemical shifts for solvents: G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg, *Organometallics*, 2010, **29**, 2176-2179.

Reactivity and Spectra

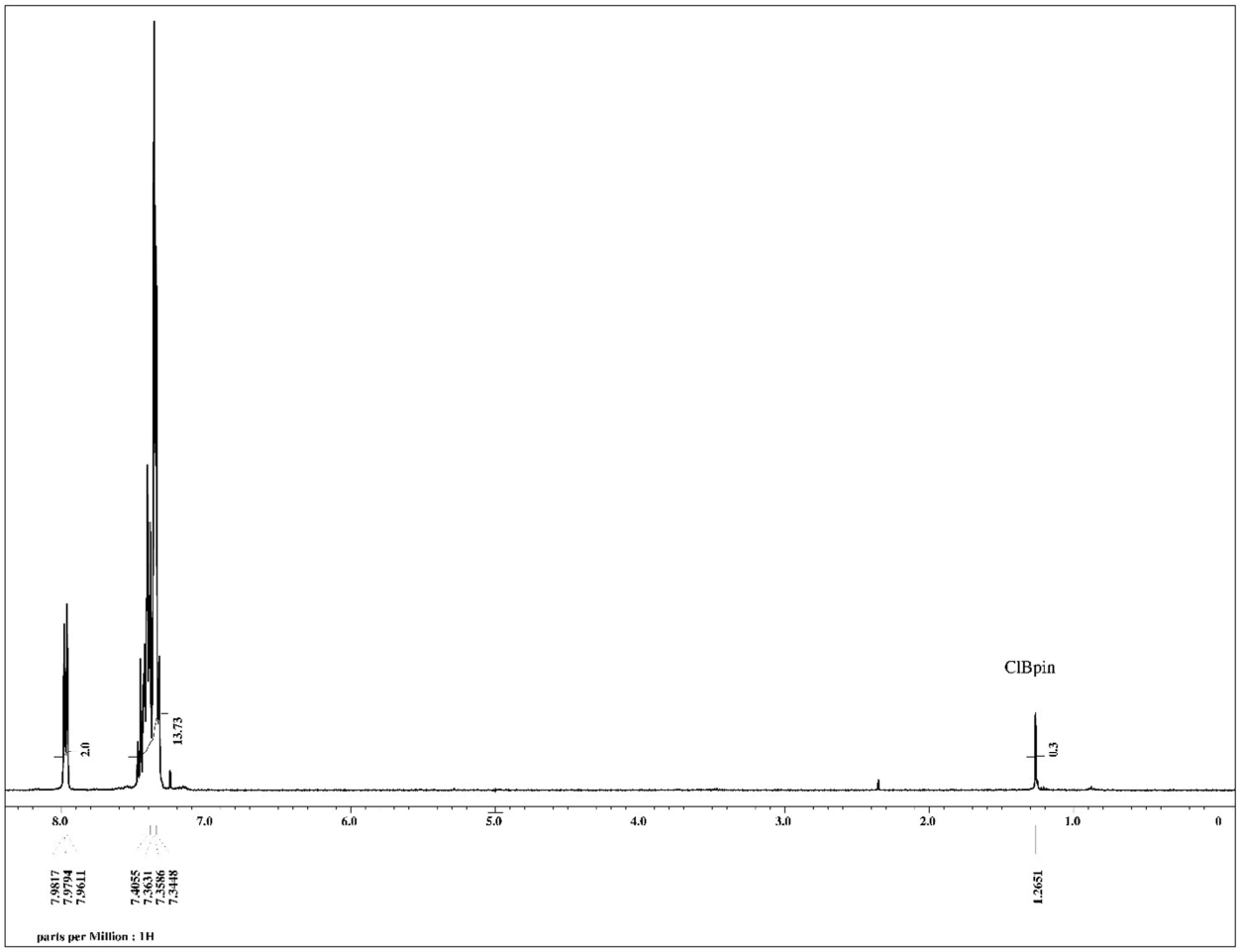

Figure S1. ^{1}H NMR spectrum of (diphenylphosphino)(phenyl)methanone, $PhC(O)PPh_2$, **1a** in $CDCl_3$.

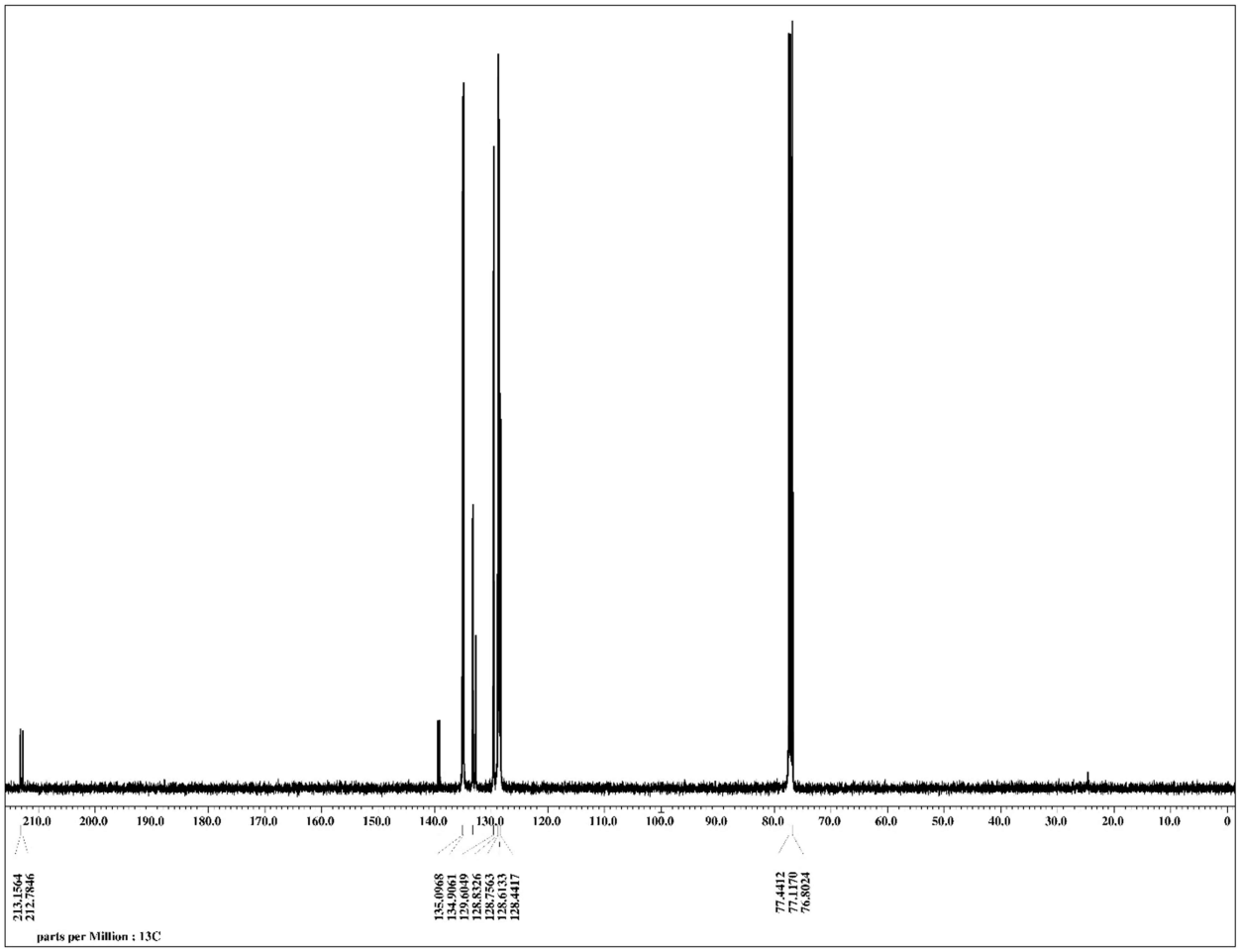

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of (diphenylphosphino)(phenyl)methanone, $PhC(O)PPh_2$, **1a** in $CDCl_3$.

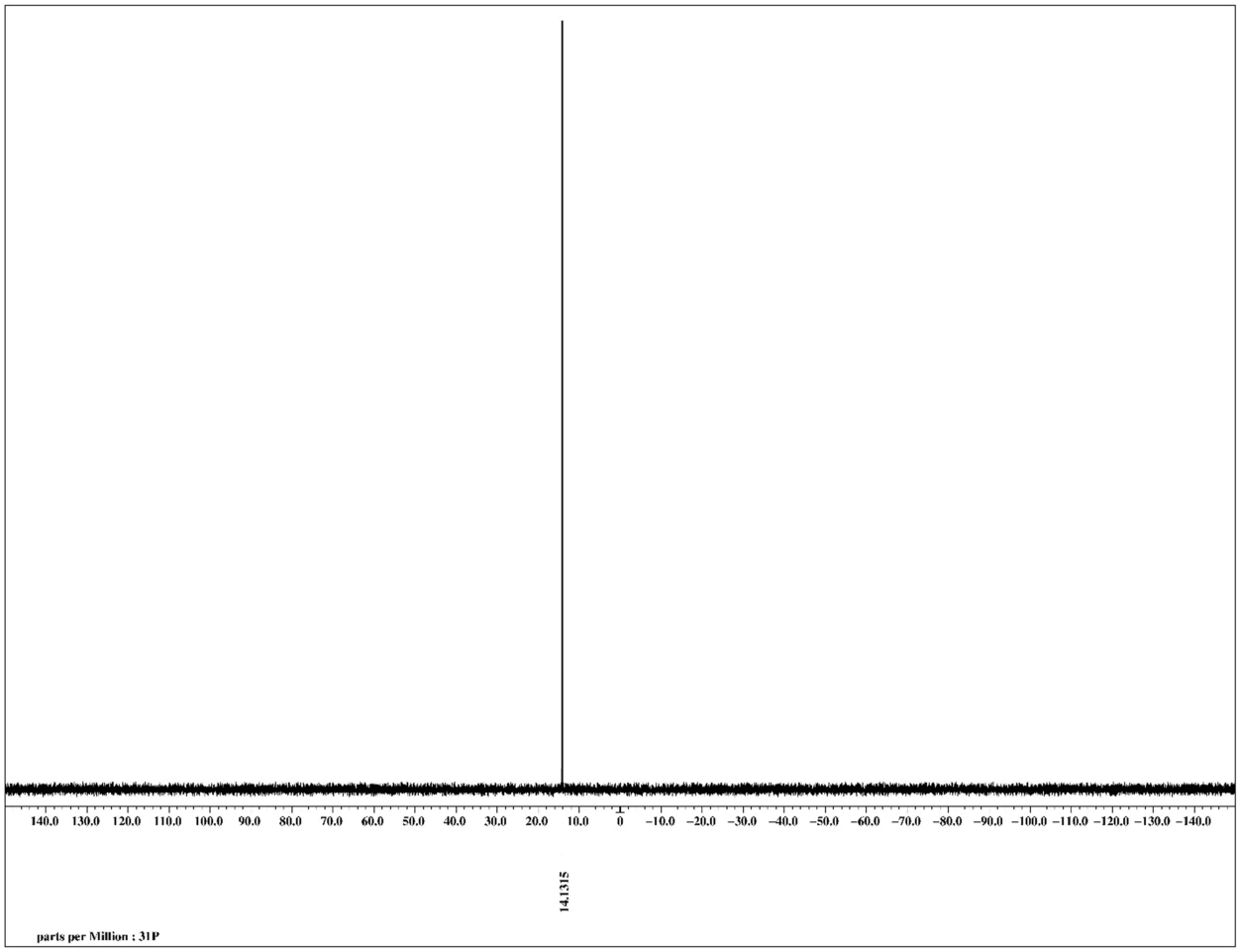

Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum of (diphenylphosphino)(phenyl)methanone, $PhC(O)PPh_2$, **1a** in $CDCl_3$.

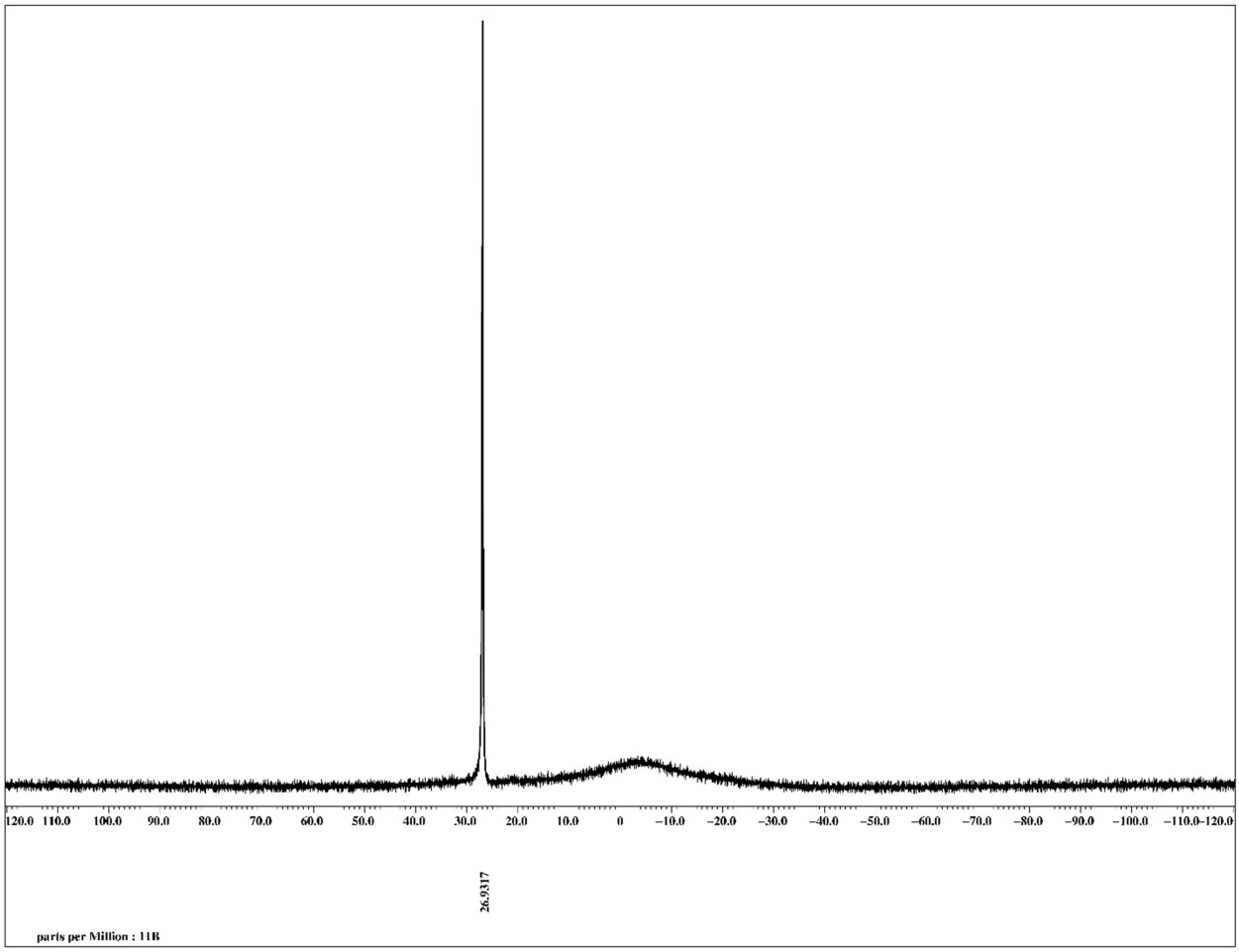

Figure S4. ^{11}B NMR spectrum of PhC(O)Cl + Ph_2PBpin in C_6D_6.

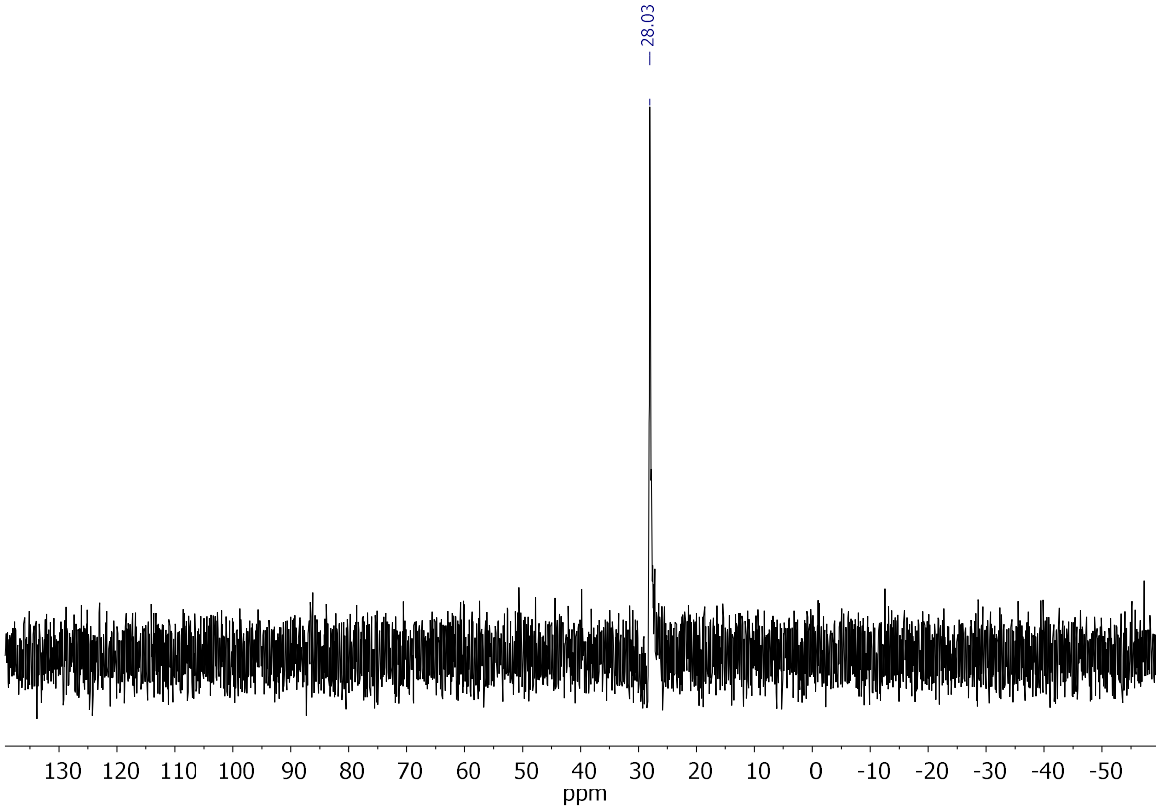

Figure S5. ^{11}B NMR spectrum of PhC(O)Cl + Ph_2PBcat in C_6D_6.

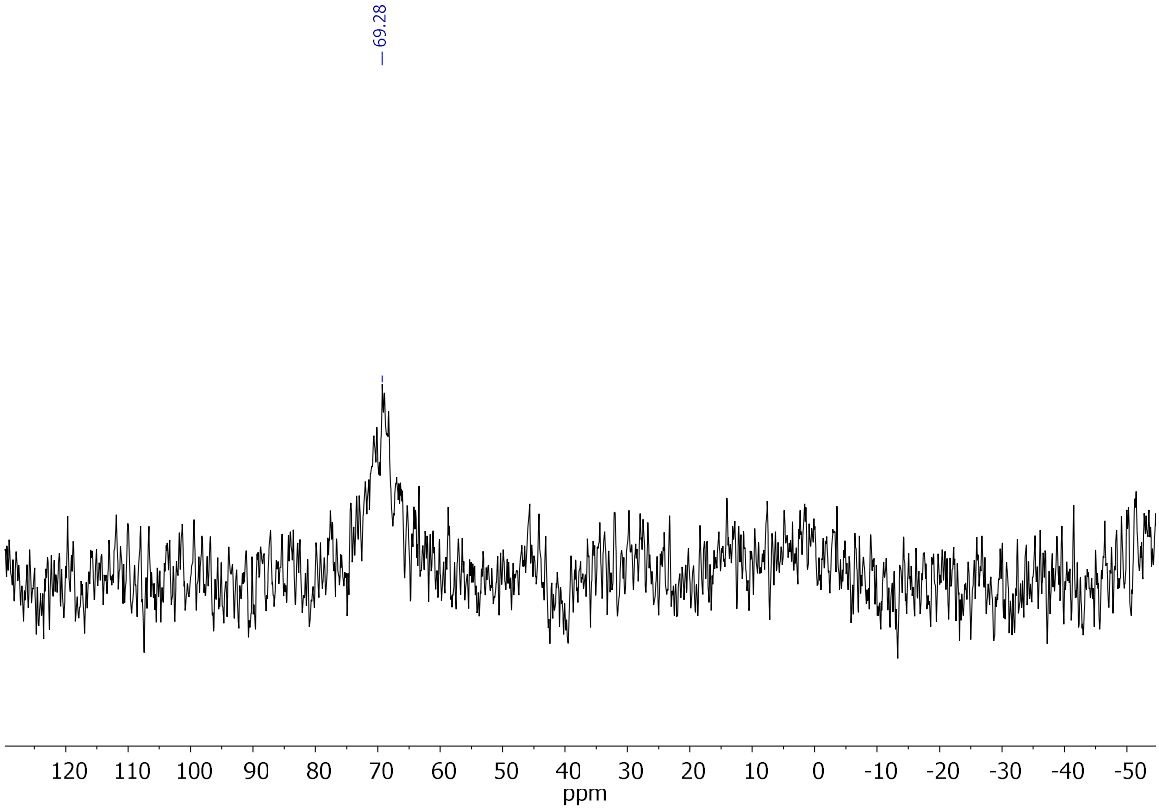

Figure S6. ^{11}B NMR spectrum of PhC(O)Cl + Ph_2PBMes_2 in C_6D_6.

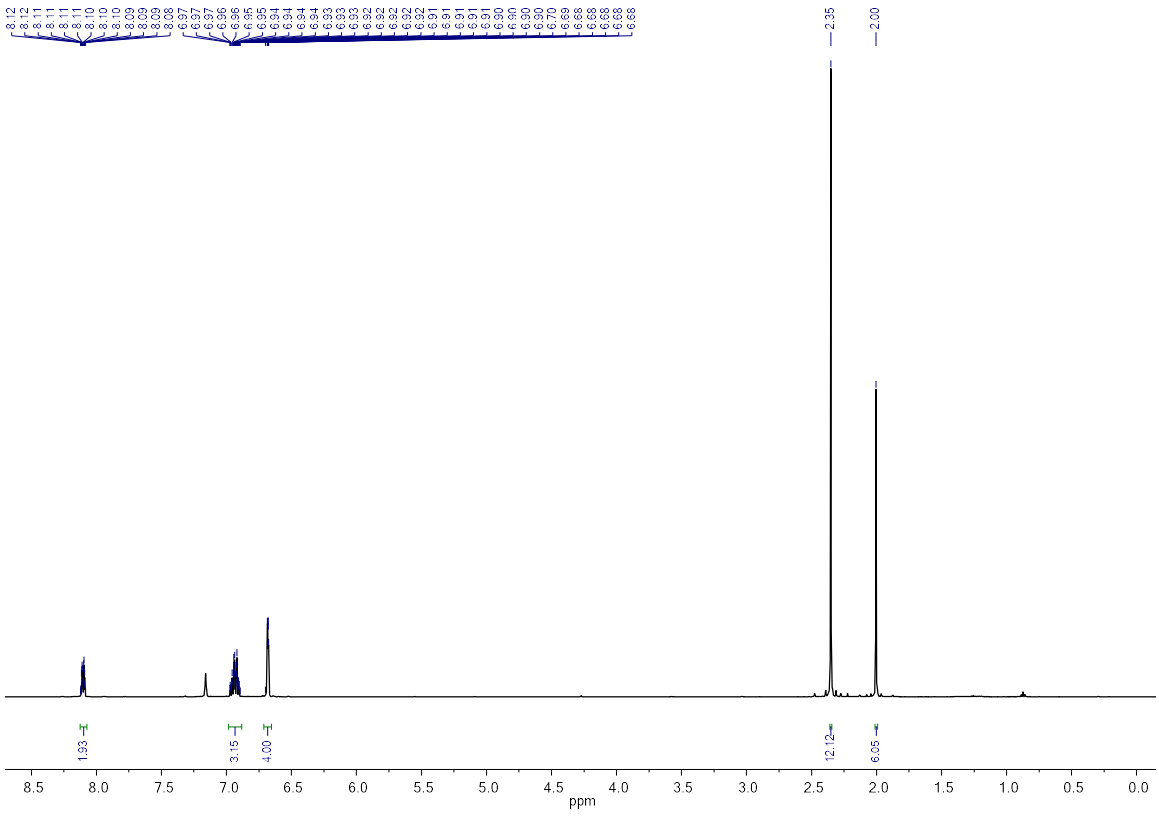

Figure S7. ^{1}H NMR spectrum of (dimesitylphosphino)(phenyl)methanone, PhC(O)PMes$_2$, **1b** in C_6D_6.

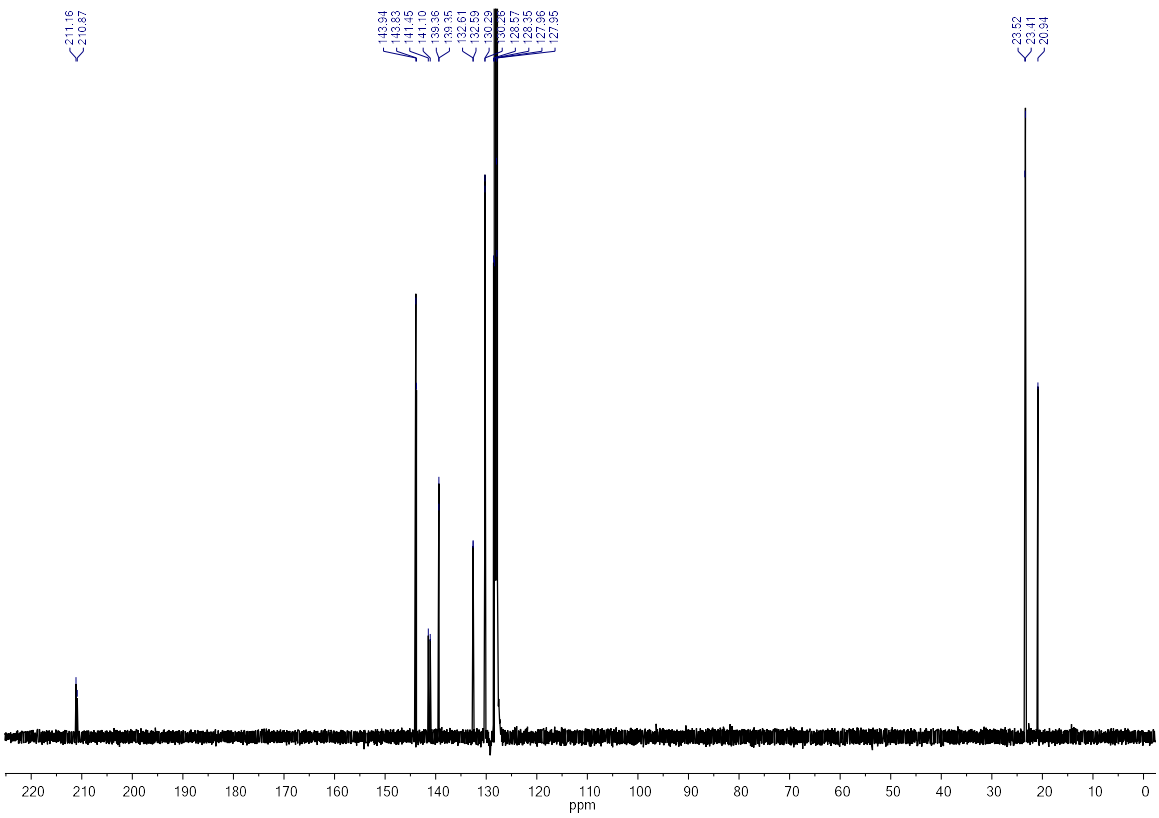

Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of (dimesitylphosphino)(phenyl)methanone, $PhC(O)PMes_2$, **1b** in C_6D_6.

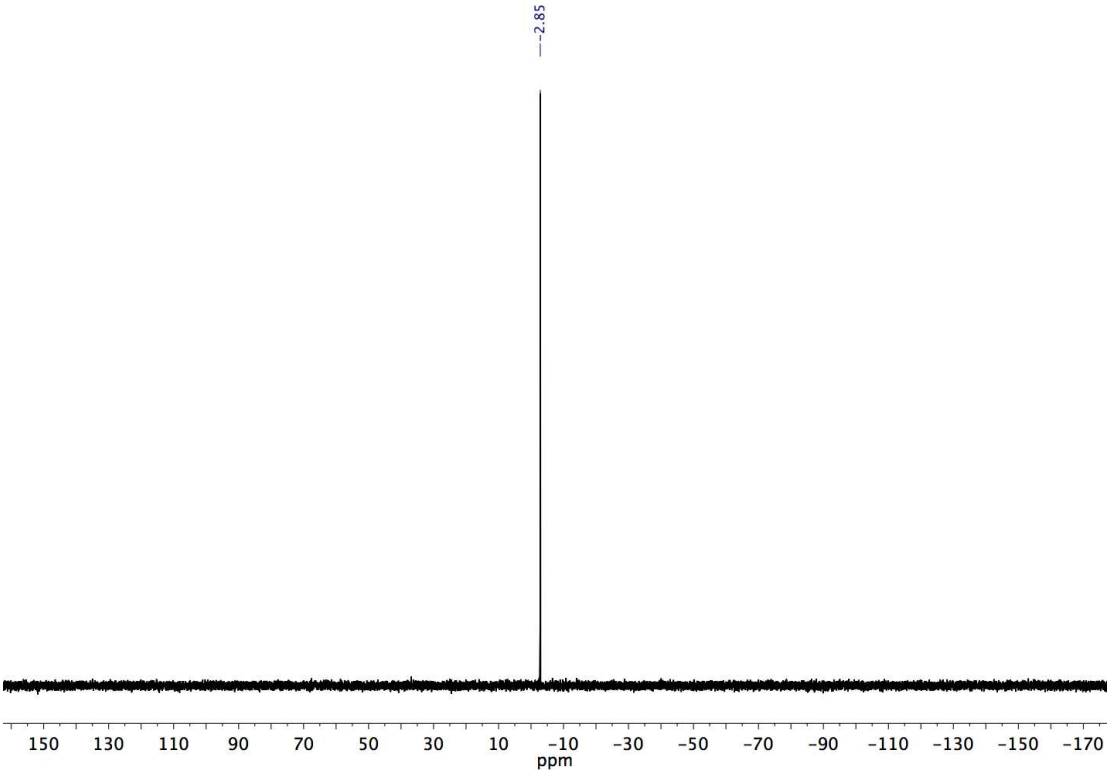

Figure S9. $^{31}P\{^{1}H\}$ NMR spectrum of (dimesitylphosphino)(phenyl)methanone, $PhC(O)PMes_2$, **1b** in C_6D_6.

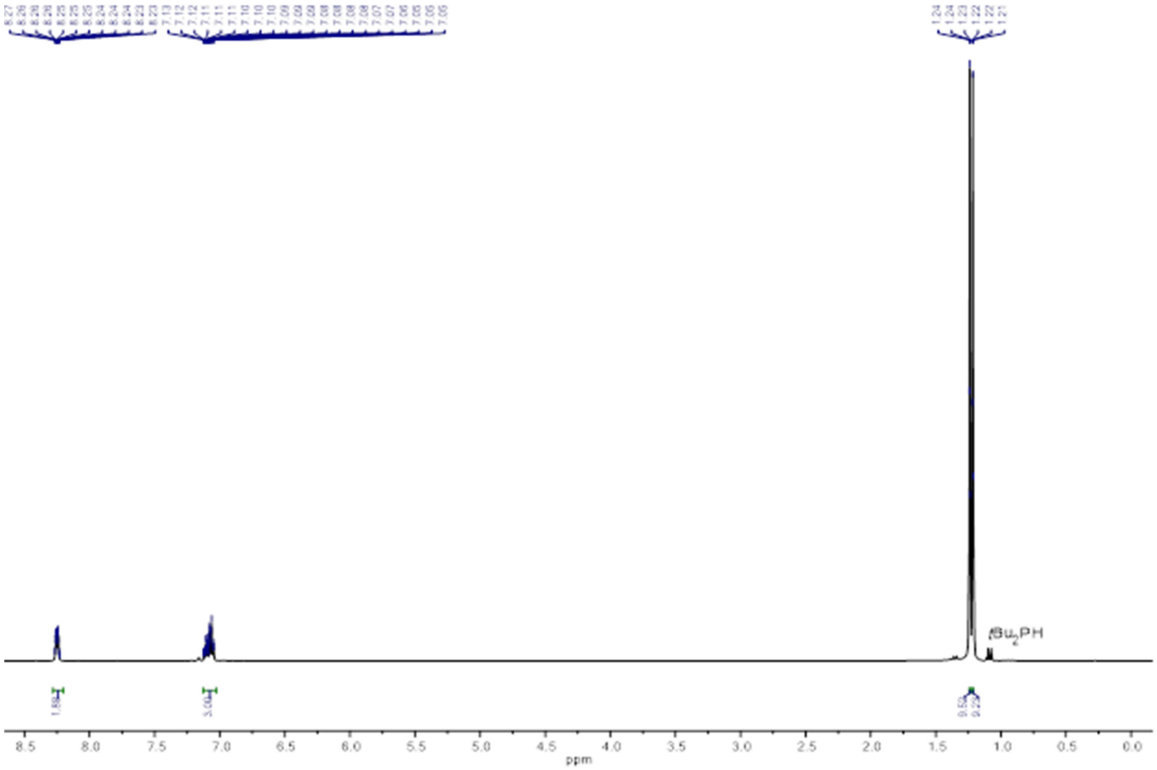

Figure S10. ^{1}H NMR spectrum of (di-*tert*-butylphosphino)(phenyl)methanone, PhC(O)P-*t*-Bu_2, **1c** in C_6D_6.

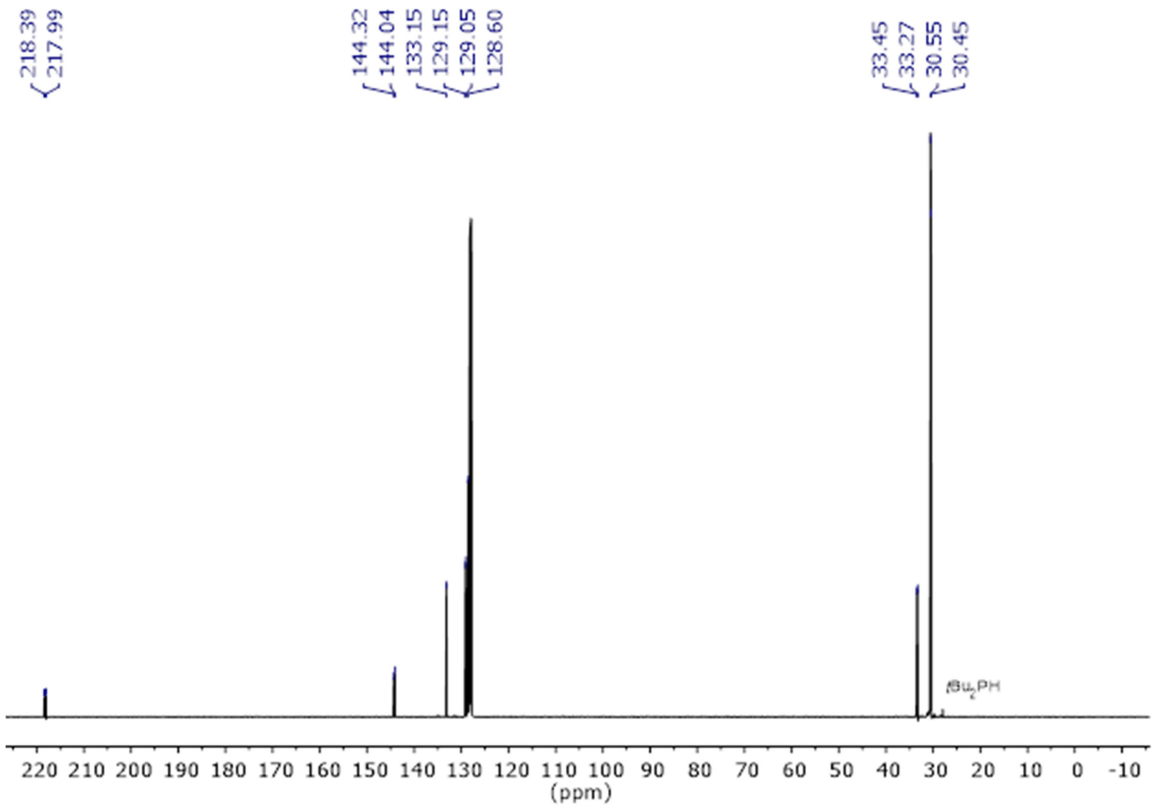

Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum of (di-*tert*-butylphosphino)(phenyl)methanone, PhC(O)P-*t*-Bu_2, **1c** in C_6D_6.

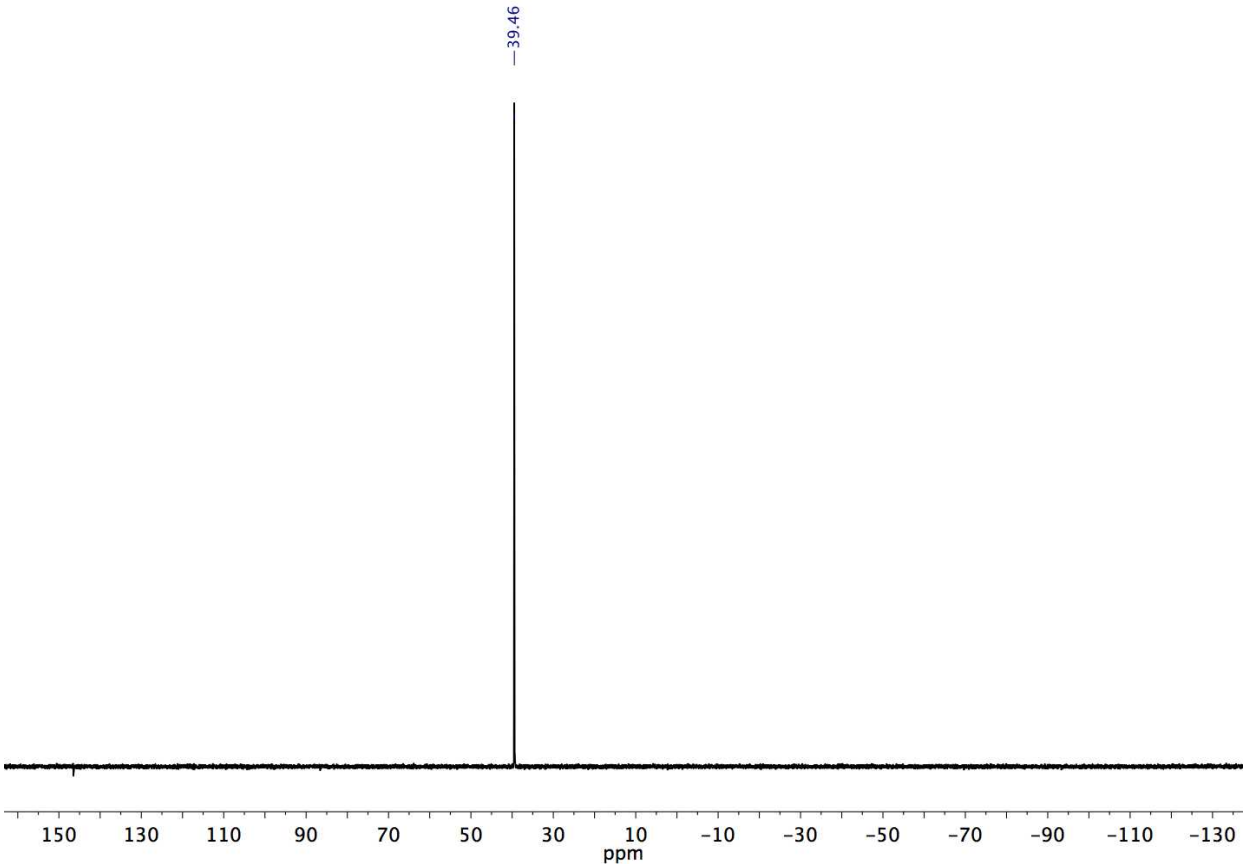

Figure S12. $^{31}P\{^{1}H\}$ NMR spectrum of (di-*tert*-butylphosphino)(phenyl)methanone, PhC(O)P-*t*-Bu_2, **1c** in C_6D_6.

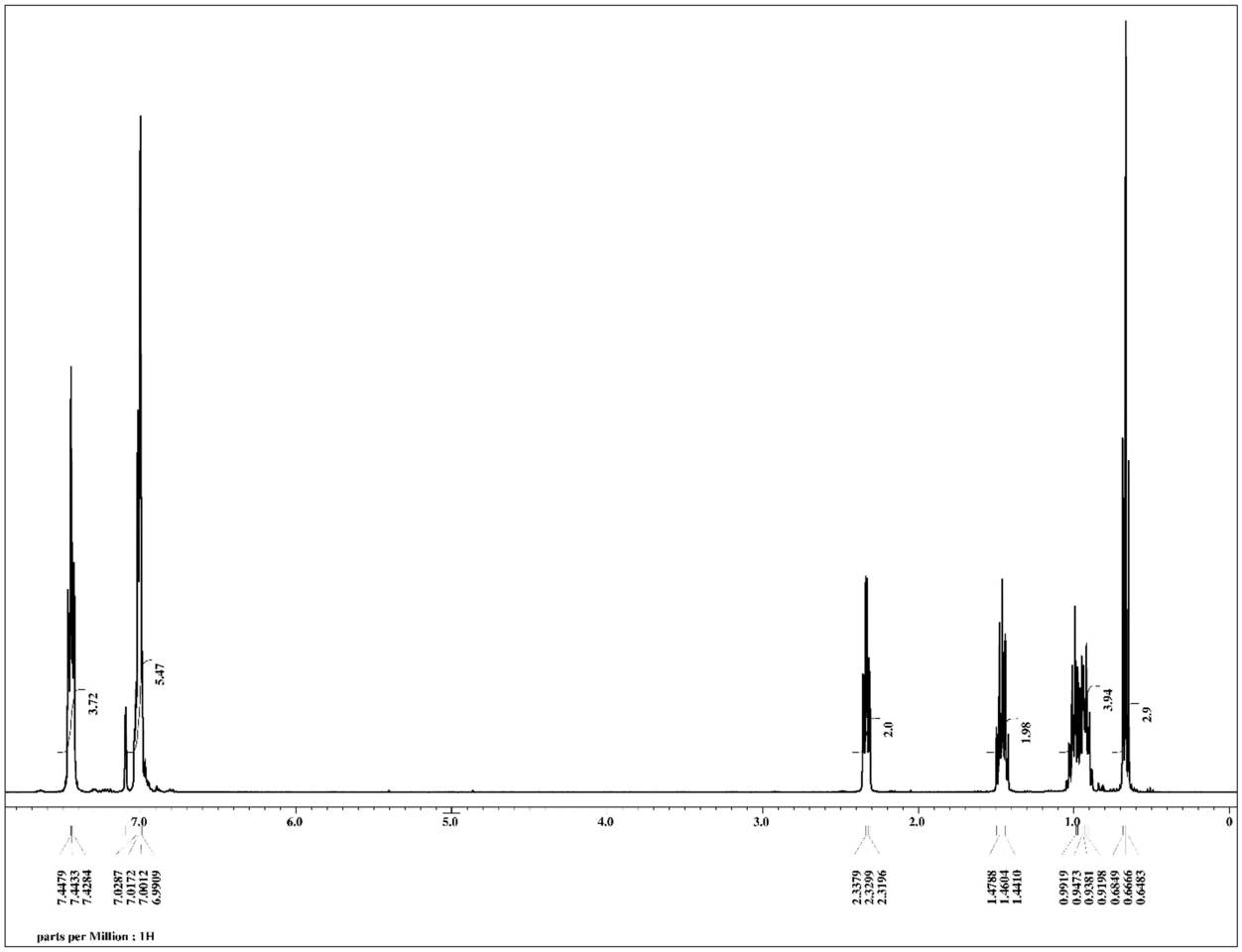

Figure S13. ^{1}H NMR spectrum of 1-(diphenylphosphino)hexan-1-one, *n*-pentylC(O)PPh_2, **1d** in C_6D_6.

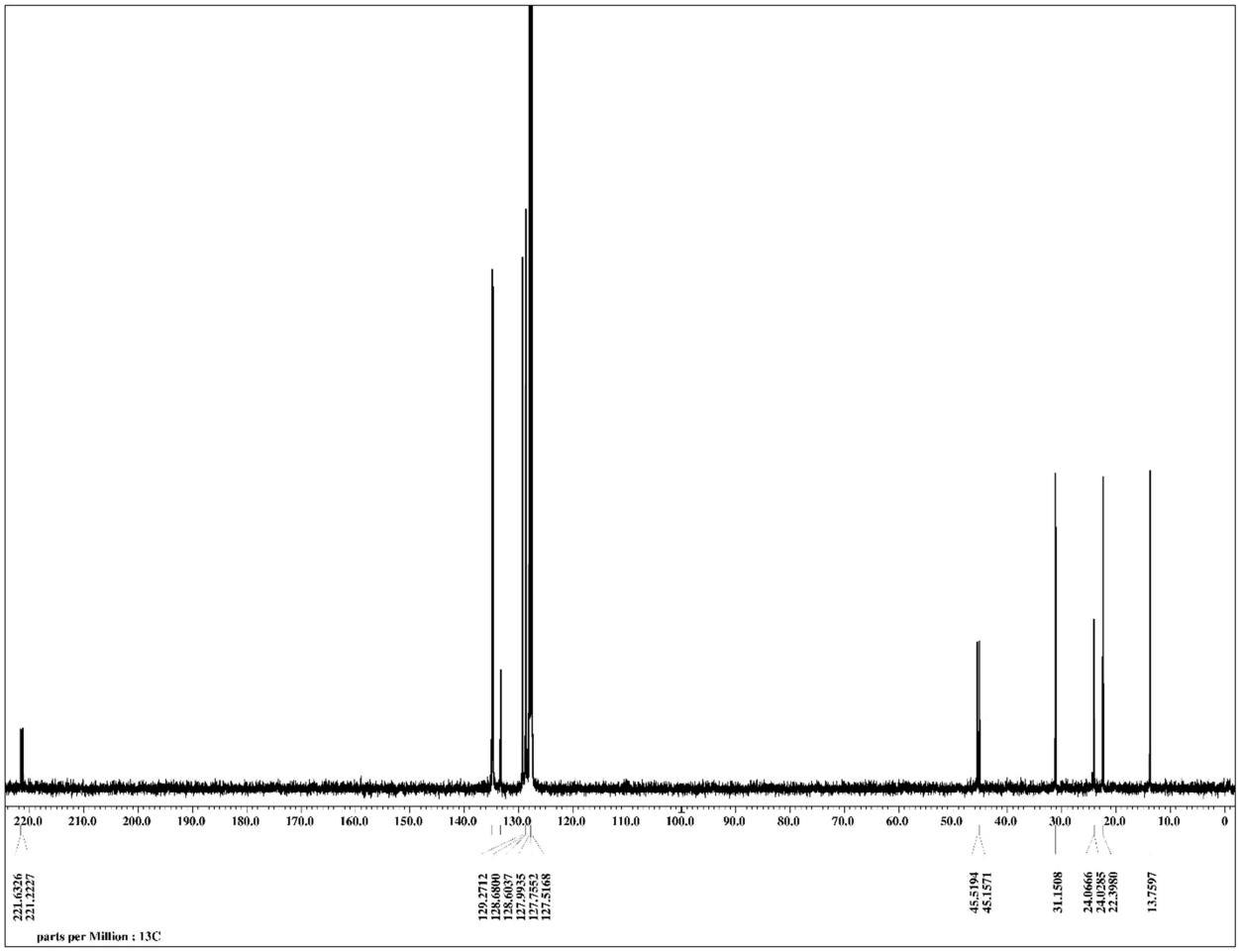

Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of 1-(diphenylphosphino)hexan-1-one, *n*-pentylC(O)PPh_2, **1d** in C_6D_6.

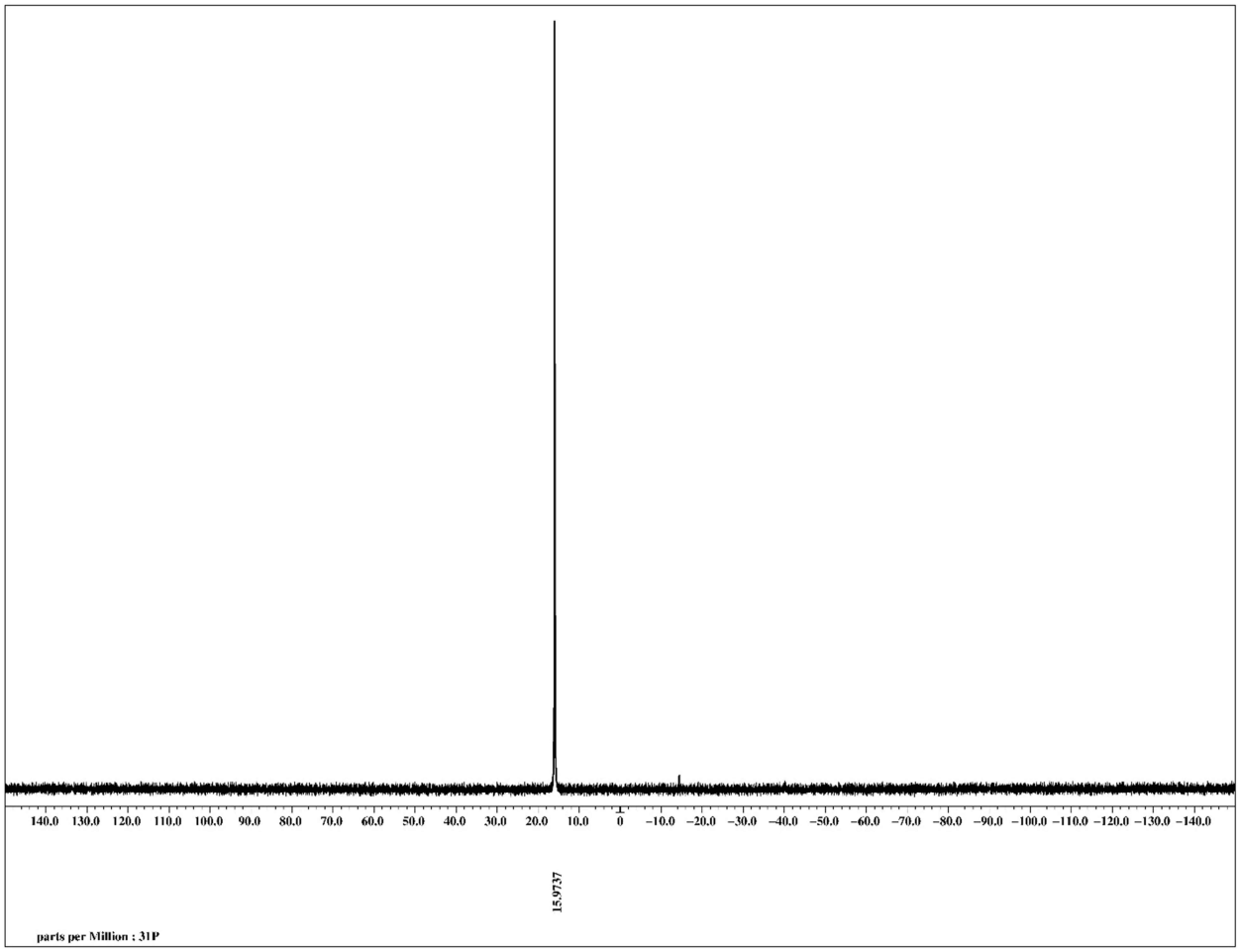

Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum of 1-(diphenylphosphino)hexan-1-one, *n*-pentylC(O)PPh_2, **1d** in C_6D_6.

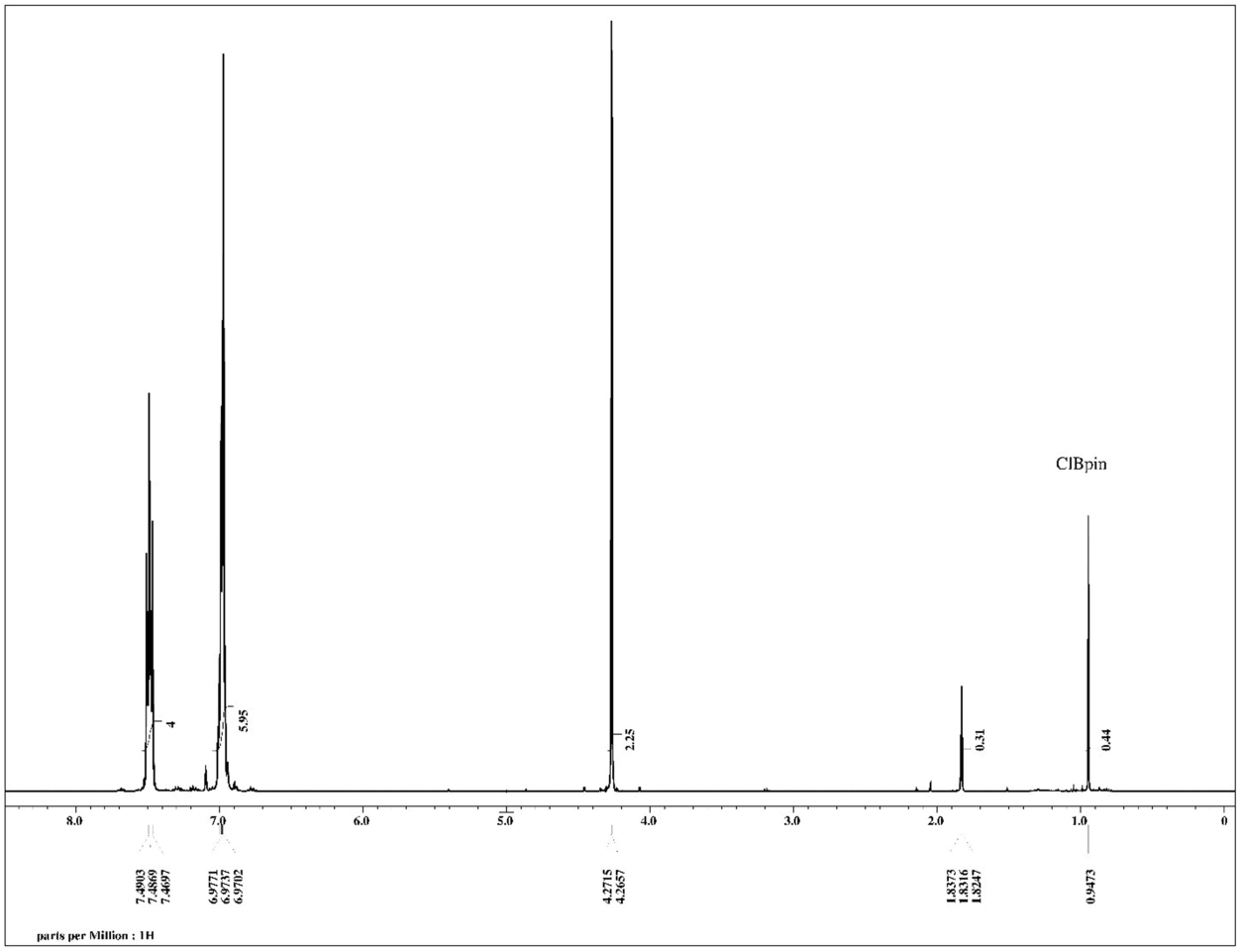

Figure S16. ^{1}H NMR spectrum of prop-2-yn-1-yl-diphenylphosphinecarboxylate, **1e** in C_6D_6.

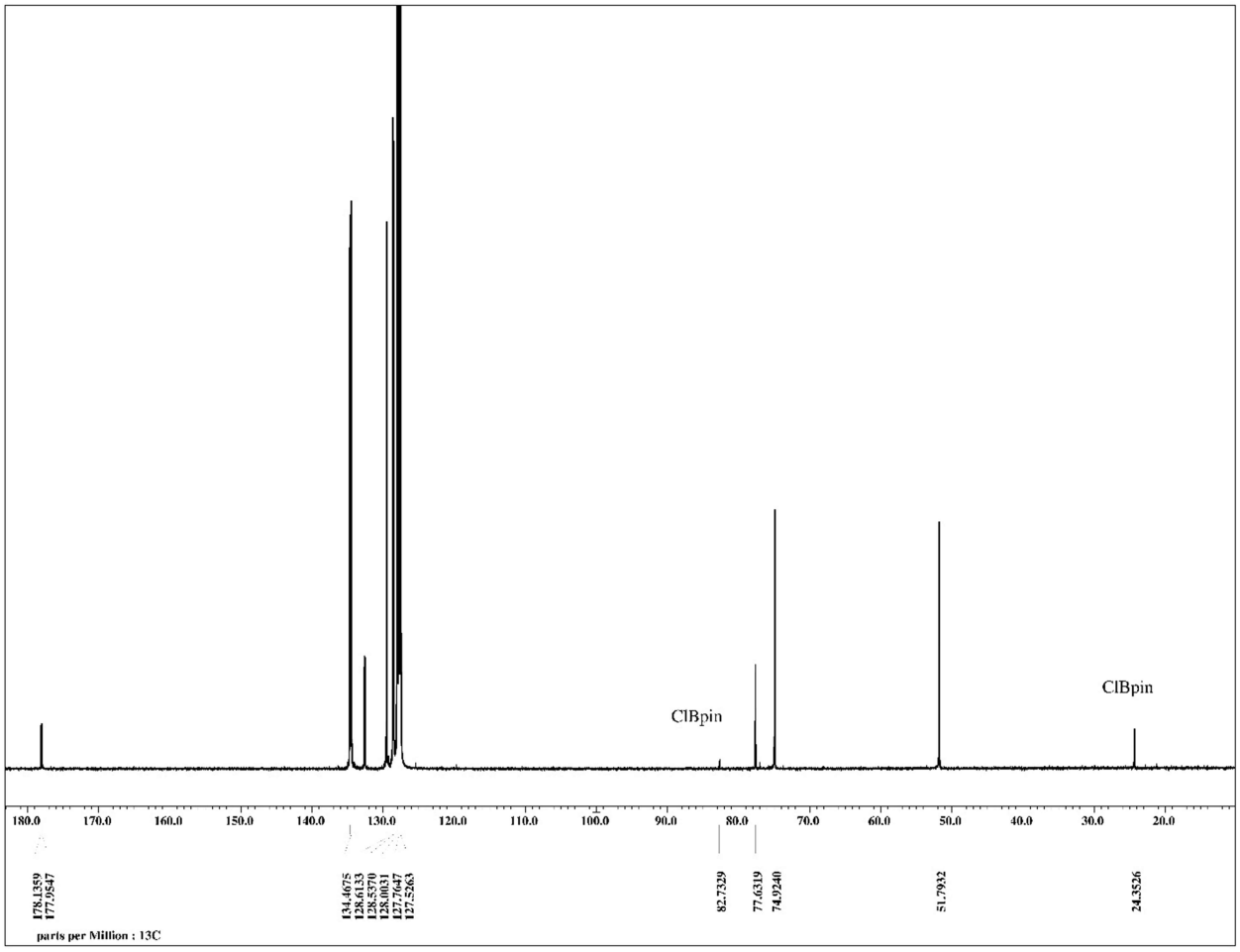

Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum of prop-2-yn-1-yl-diphenylphosphinecarboxylate, **1e** in C_6D_6.

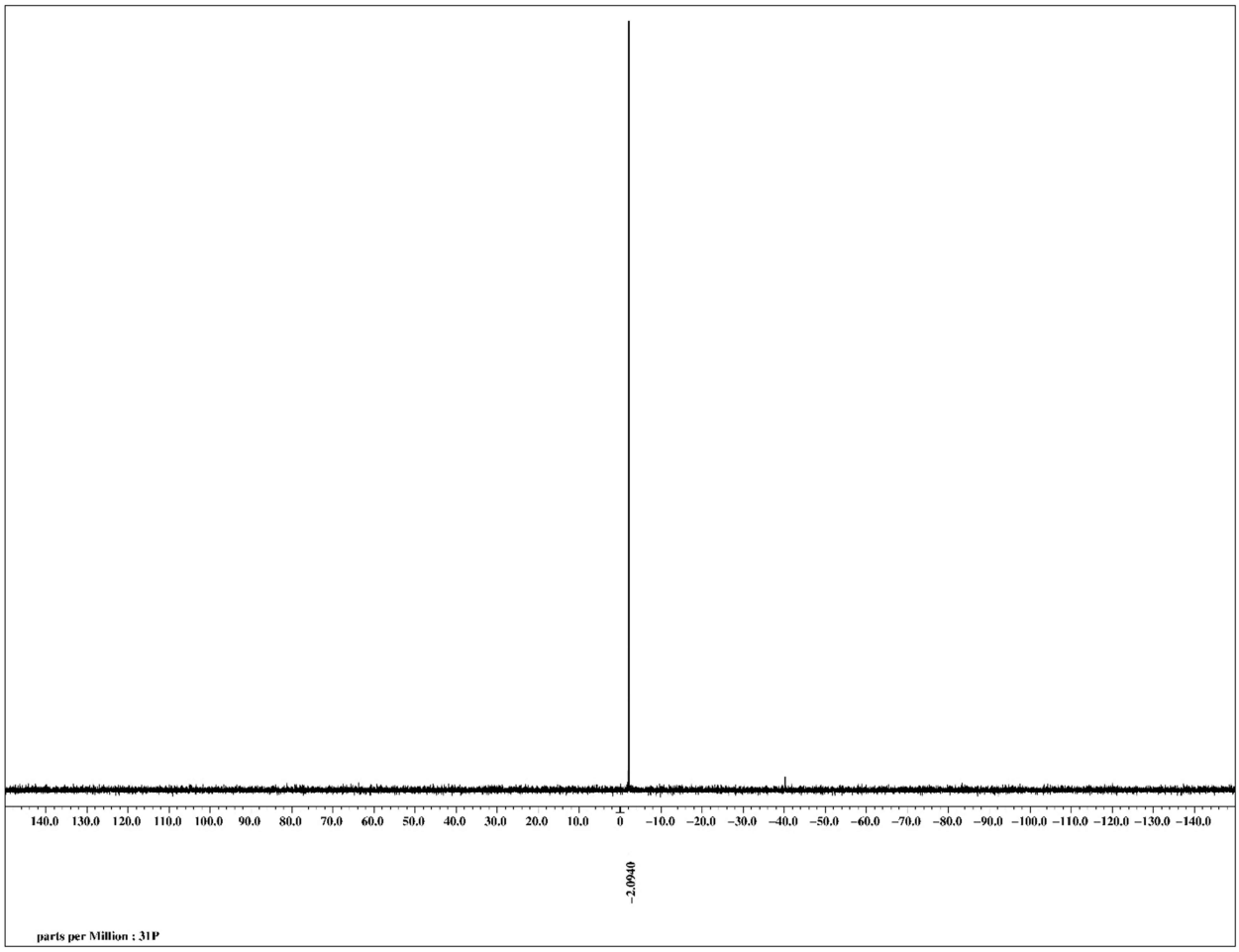

Figure S18. $^{31}P\{^{1}H\}$ NMR spectrum of prop-2-yn-1-yl-diphenylphosphinecarboxylate, **1e** in C_6D_6.

Reactivity of Ph_2PBpin (1 equiv.) and *trans*-cinnamoyl chloride.

To a stirred C_6D_6 (0.5 mL) solution of *trans*-cinnamoyl chloride (20 mg, 0.12 mmol) was added a C_6D_6 (0.5 mL) solution of Ph_2PBpin (37 mg, 0.12 mmol). The reaction was allowed to proceed for 18 h at RT at which point the reaction was analyzed by multi-nuclear NMR spectroscopy. Selected NMR data: ^{1}H NMR (400 MHz, C_6D_6) δ: 7.72-7.62 (ov m, Ar), 7.51 (m, Ar), 7.41 (d, J_{HH} = 15.1 Hz, *H*C=CH, **1f**), 7.29 (m, Ar), 7.15-6.73 (ov m, Ar), 6.15 (d, J_{HH} = 15.1 Hz, HC=C*H,* **1f**), 5.99 (d ov dd, J_{HH} = 10.5 Hz, J_{HP} = 6.9, 6.9 Hz), 4.96 (dd, J_{HH} = 10.5 Hz, J_{HP} = 2.8 Hz), 4.80 (dd, J_{HH} = 10.1 Hz, J_{HP} = 3.2 Hz), 1.03 (s), 0.84 (s, ClBpin), 0.80 (s), 0.74 (s); ^{11}B NMR (128 MHz, C_6D_6) δ: 27.1 (sharp, ClBpin), 22 (br), 21 (br); ^{31}P{^{1}H} NMR (162 MHz, C_6D_6) δ: 82.7, 17.5, 7.2, 3.2, 0.3, -0.1, -1.1, -2.9, -16.8.

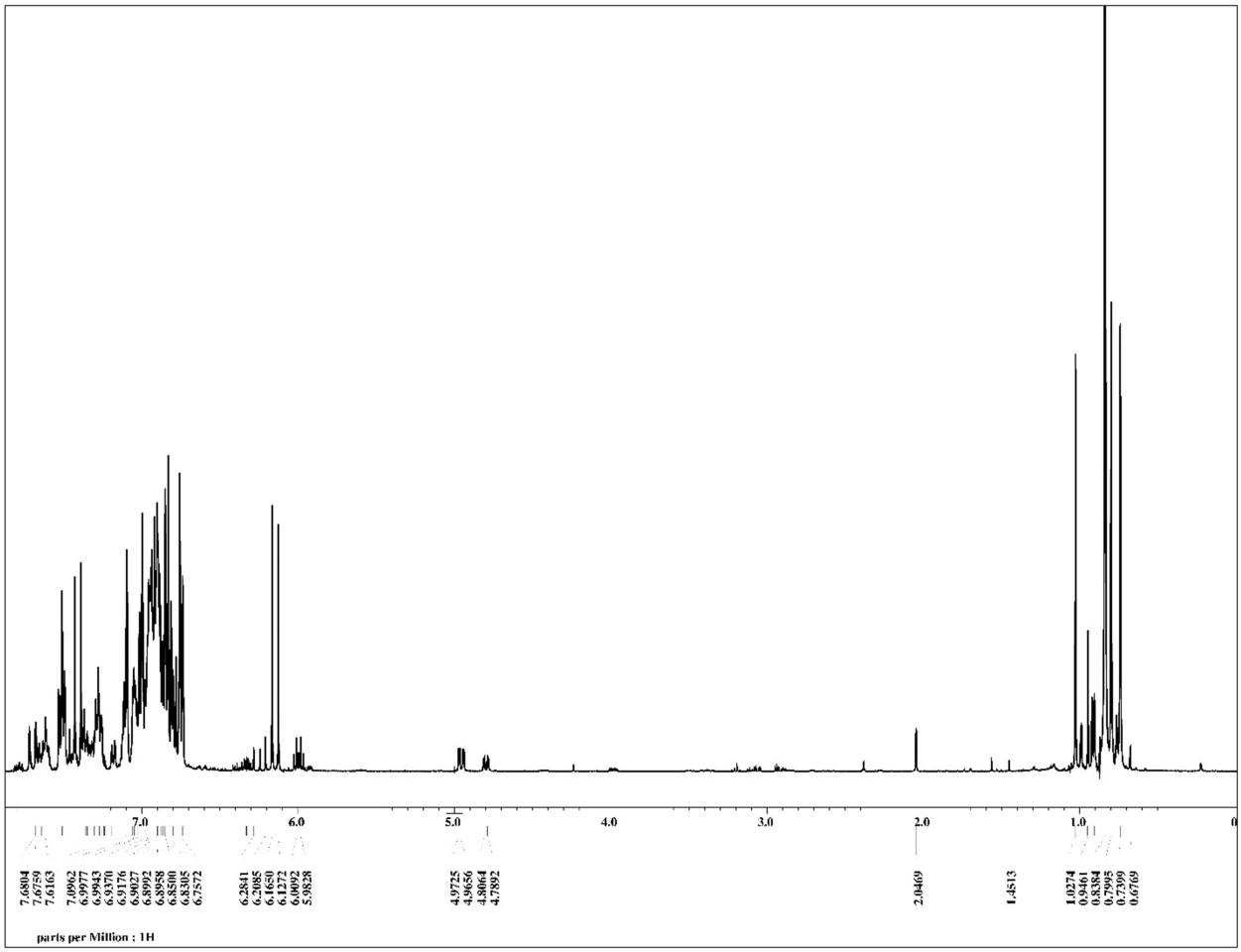

Figure S19. ^{1}H NMR spectrum of Ph_2PBpin (1 eq) + *trans*-cinnamoyl chloride in C_6D_6.

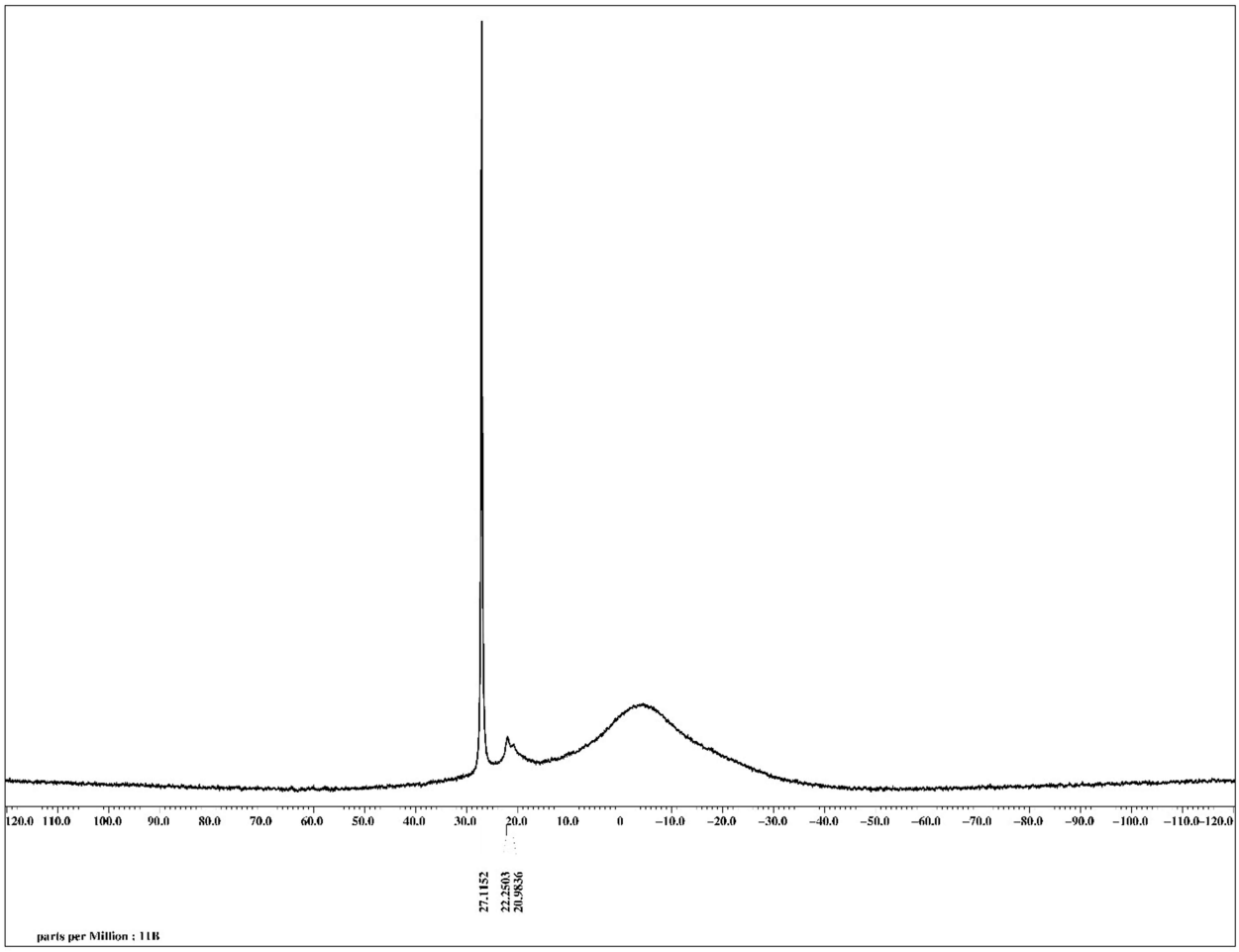

Figure S20. ^{11}B NMR spectrum of Ph_2PBpin (1 eq) + *trans*-cinnamoyl chloride in C_6D_6.

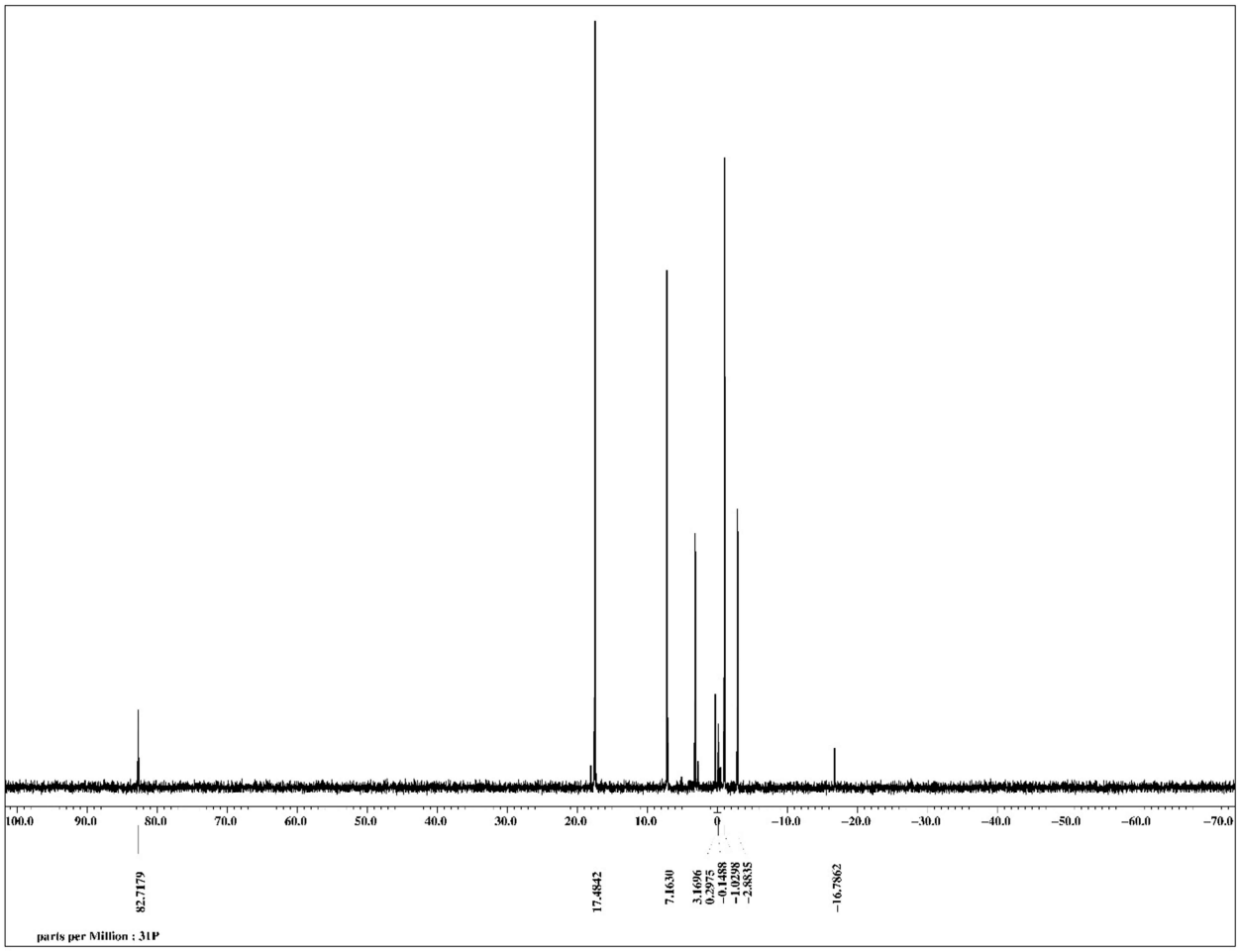

Figure S21. $^{31}P\{^{1}H\}$ NMR spectrum of Ph_2PBpin (1 eq) + *trans*-cinnamoyl chloride in C_6D_6.

Reactivity of Ph_2PBpin (2 equiv.) and *trans*-cinnamoyl chloride.

To a stirred C_6D_6 (0.5 mL) solution of *trans*-cinnamoyl chloride (20 mg, 0.12 mmol) was added a C_6D_6 (0.5 mL) solution of Ph_2PBpin (75 mg, 0.24 mmol). The reaction was allowed to proceed for 18 h at RT at which point the reaction was analyzed by multi-nuclear NMR spectroscopy. Selected NMR data: ^1H NMR (400 MHz, C_6D_6) δ: 7.98 (m, Ar), 7.75 (m, Ar), 7.68 (t, J_{HH} = 7.8 Hz, Ar), 7.61 (m, Ar), 7.37 (m, Ar), 7.27 (m, Ar), 7.12-6.85 (ov m, Ar), 6.54 (dt, J_{HH} = 15.6 Hz, J_{HP} = 4.6 Hz), 6.27 (d, J_{HH} = 16.0 Hz), 5.99 (d ov dd, J_{HH} = 10.5 Hz, J_{HP} = 6.9, 6.9 Hz), 4.96 (dd, J_{HH} = 10.5 Hz, J_{HP} = 2.8 Hz), 0.84 (s, ClBpin), 0.80 (s), 0.74 (s), 0.73 (s); ^{11}B NMR (128 MHz, C_6D_6) δ: 35 (br, Ph_2PBpin), 27.0 (sharp, ClBpin), 21 (br); $^{31}P\{^1H\}$ NMR (162 MHz, C_6D_6) δ: 10.7, 7.2, -1.1, -14.4, -16.8, -40.1 ($HPPh_2$), -63.4 (br, Ph_2PBpin).

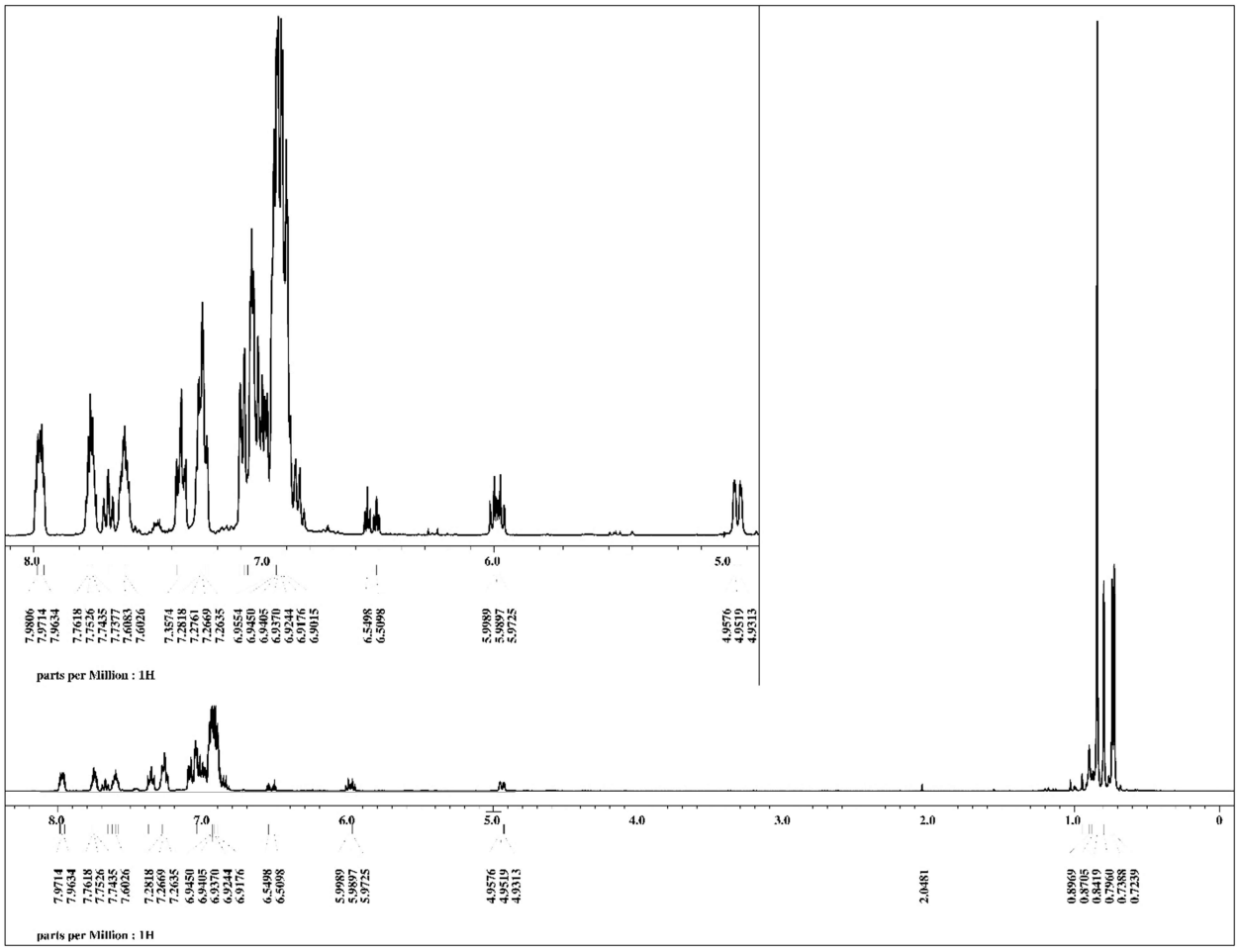

Figure S22. ^1H NMR spectrum of Ph_2PBpin (2 eq) and *trans*-cinnamoyl chloride in C_6D_6.

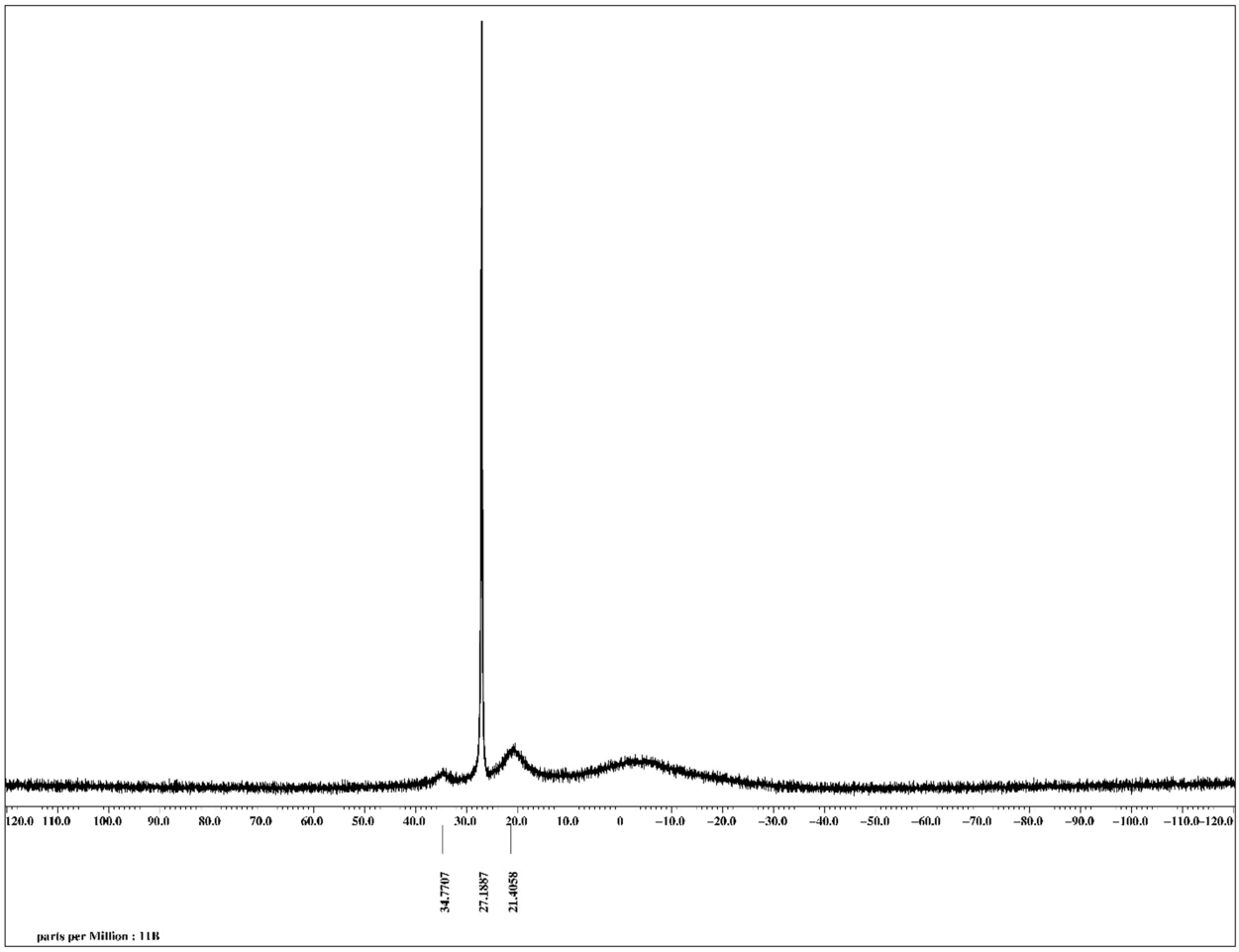

Figure S23. ^{11}B NMR spectrum of Ph_2PBpin (2 eq) and *trans*-cinnamoyl chloride in C_6D_6.

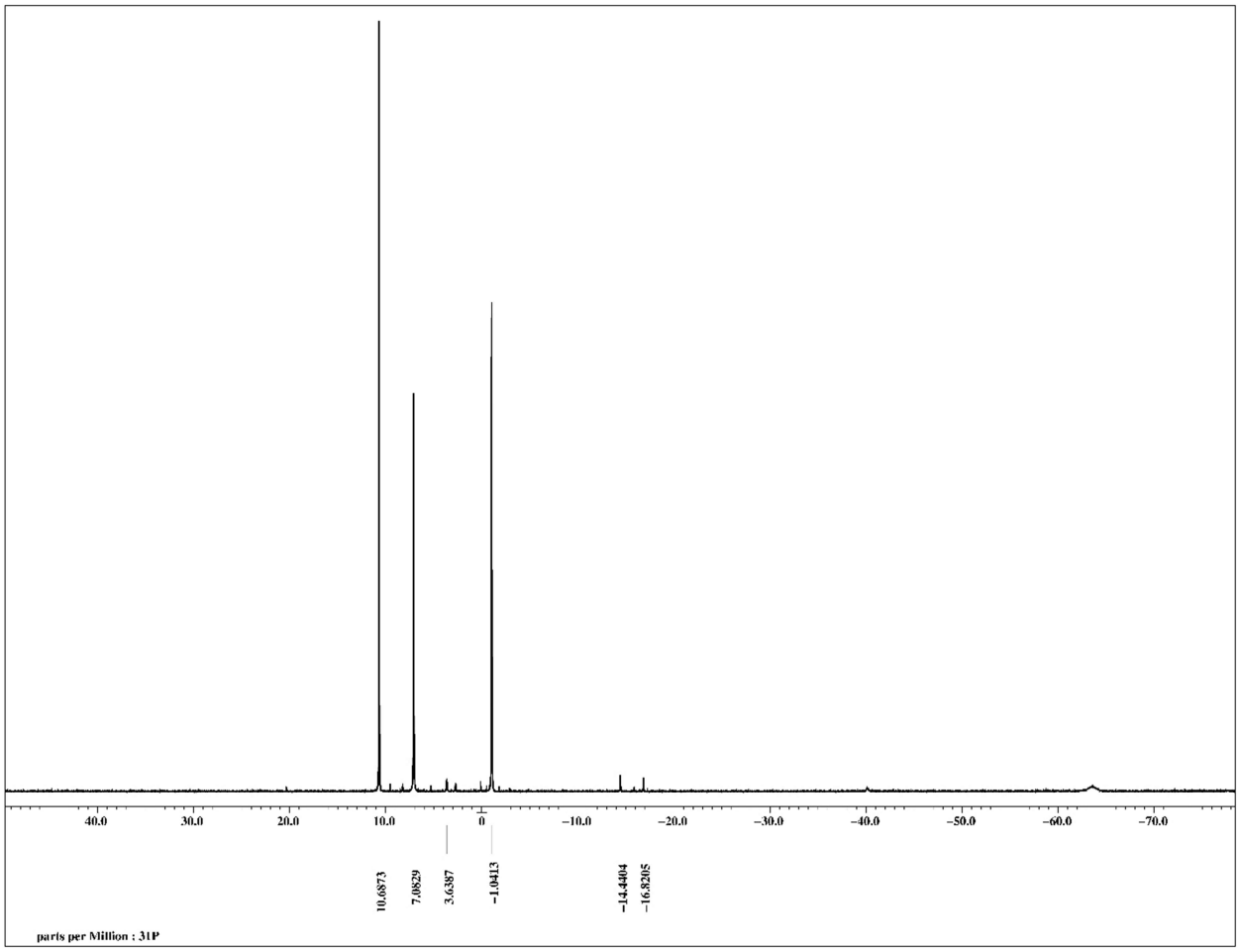

Figure S24. $^{31}P\{^{1}H\}$ NMR spectrum of Ph_2PBpin (2 eq) and *trans*-cinnamoyl chloride in C_6D_6.

Reactivity of Ph_2PBpin (1 equiv.) and 9-fluorenone-4-carbonyl chloride.

To a stirred C_6D_6 (0.5 mL) solution of 9-fluorenone-4-carbonyl chloride (15 mg, 0.06 mmol) was added a C_6D_6 (0.5 mL) solution of Ph_2PBpin (19 mg, 0.06 mmol). The reaction was allowed to proceed for 18 h at RT at which point the reaction mixture was analyzed by multinuclear NMR spectroscopy. Selected NMR data: ^1H NMR (400 MHz, C_6D_6) δ: 8.02 (m, Ar), 7.92 (d, J_{HH} = 7.8 Hz, Ar), 7.88 (m, Ar), 7.71 (m, Ar), 7.55-7.29 (ov m, Ar), 6.95-6.82 (ov m, Ar), 6.77 (m, Ar), 6.66 (m, Ar), 6.45 (t, J_{HH} = 7.3 Hz, Ar), 0.83 (s, ClBpin), 0.63 (s); ^{11}B NMR (128 MHz, C_6D_6) δ: 27.2 (sharp, ClBpin), 22 (br), 21 (br); $^{31}P\{^1H\}$ NMR (162 MHz, C_6D_6) δ: 25.5, 22.1, 20.3, 18.0, -40.2 (minor, $HPPh_2$).

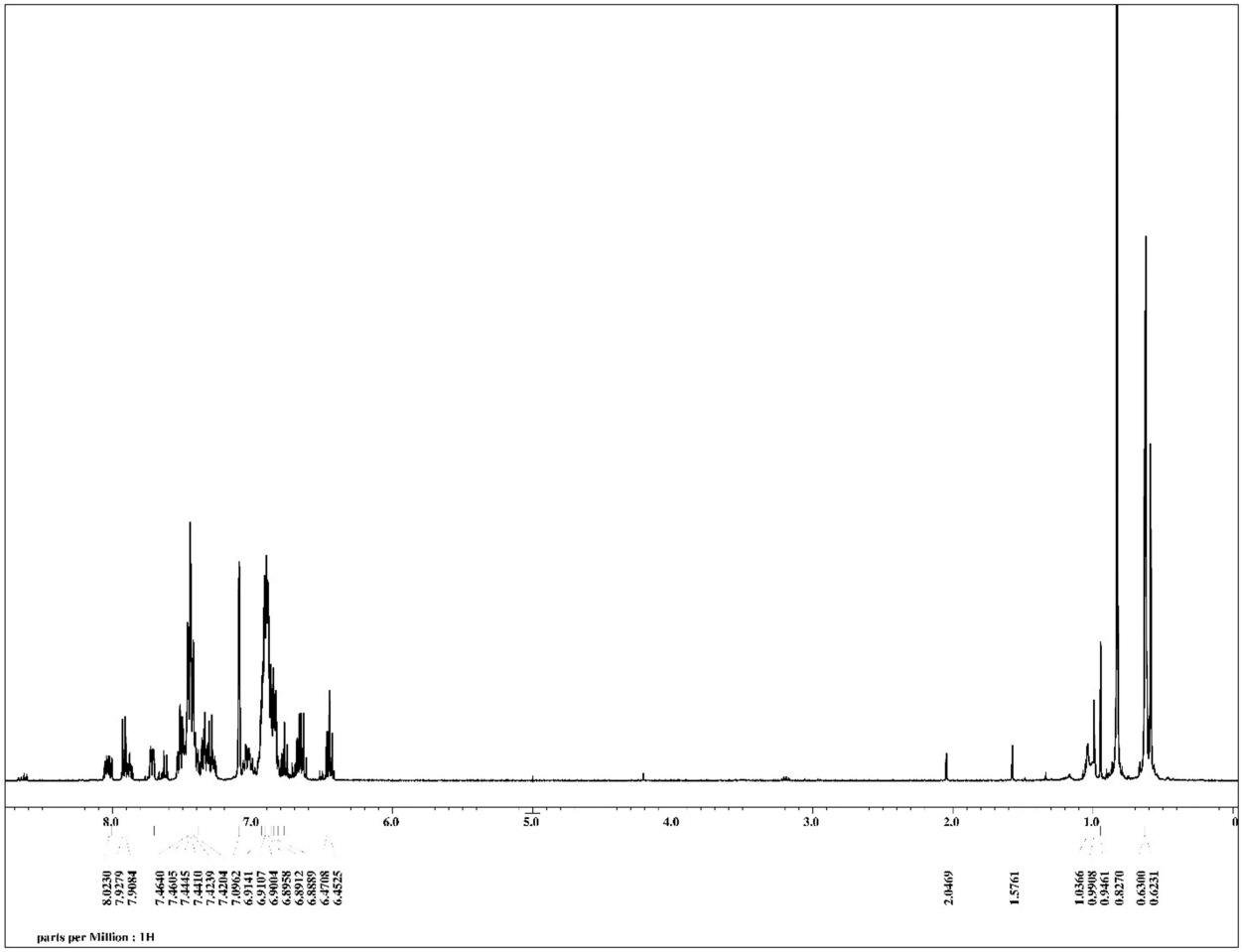

Figure S25. ^1H NMR spectrum of Ph_2PBpin (1 eq) + 9-fluorenone-4-carbonyl chloride in C_6D_6.

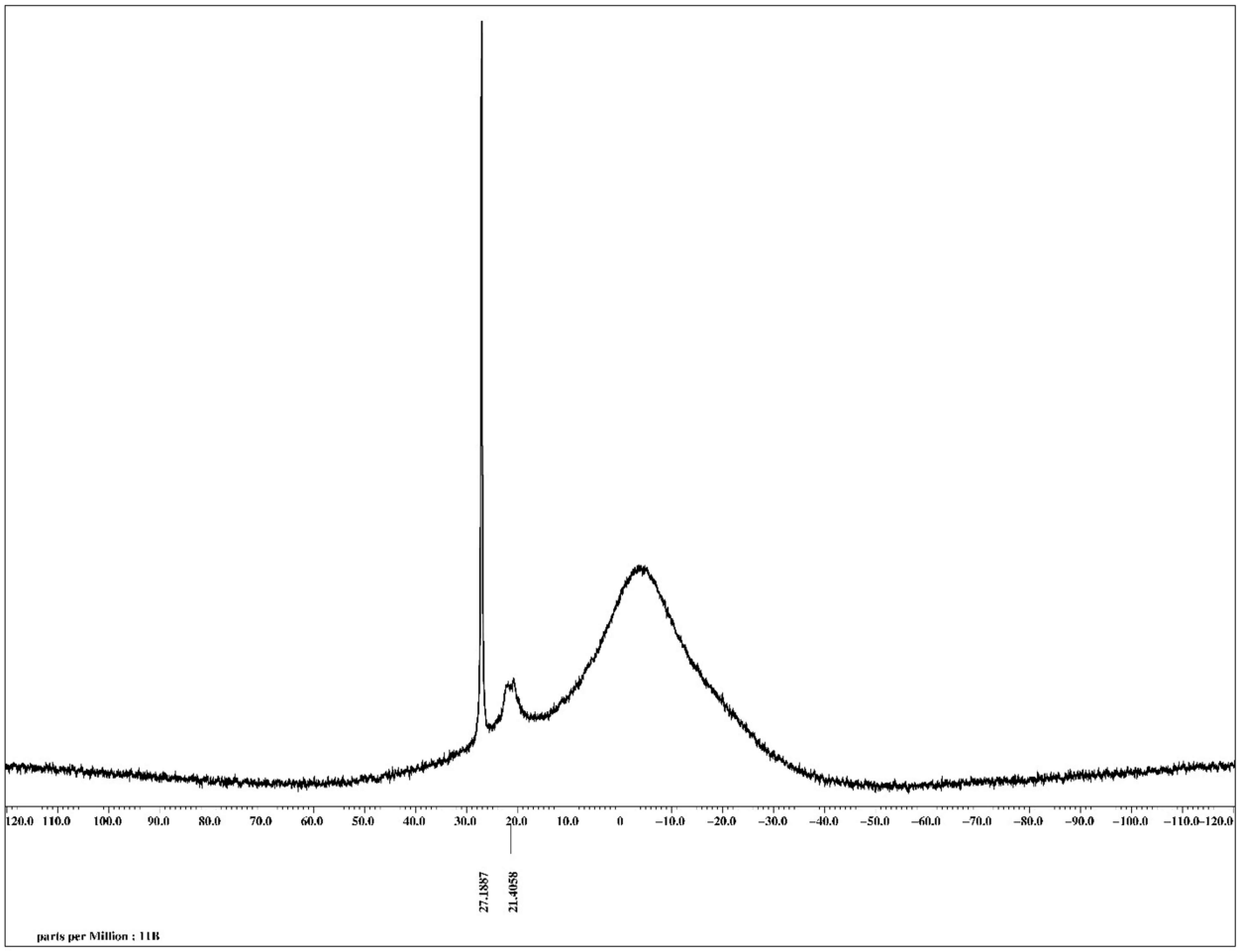

Figure S26. ^{11}B NMR spectrum of Ph_2PBpin (1 eq) + 9-fluorenone-4-carbonyl chloride in C_6D_6.

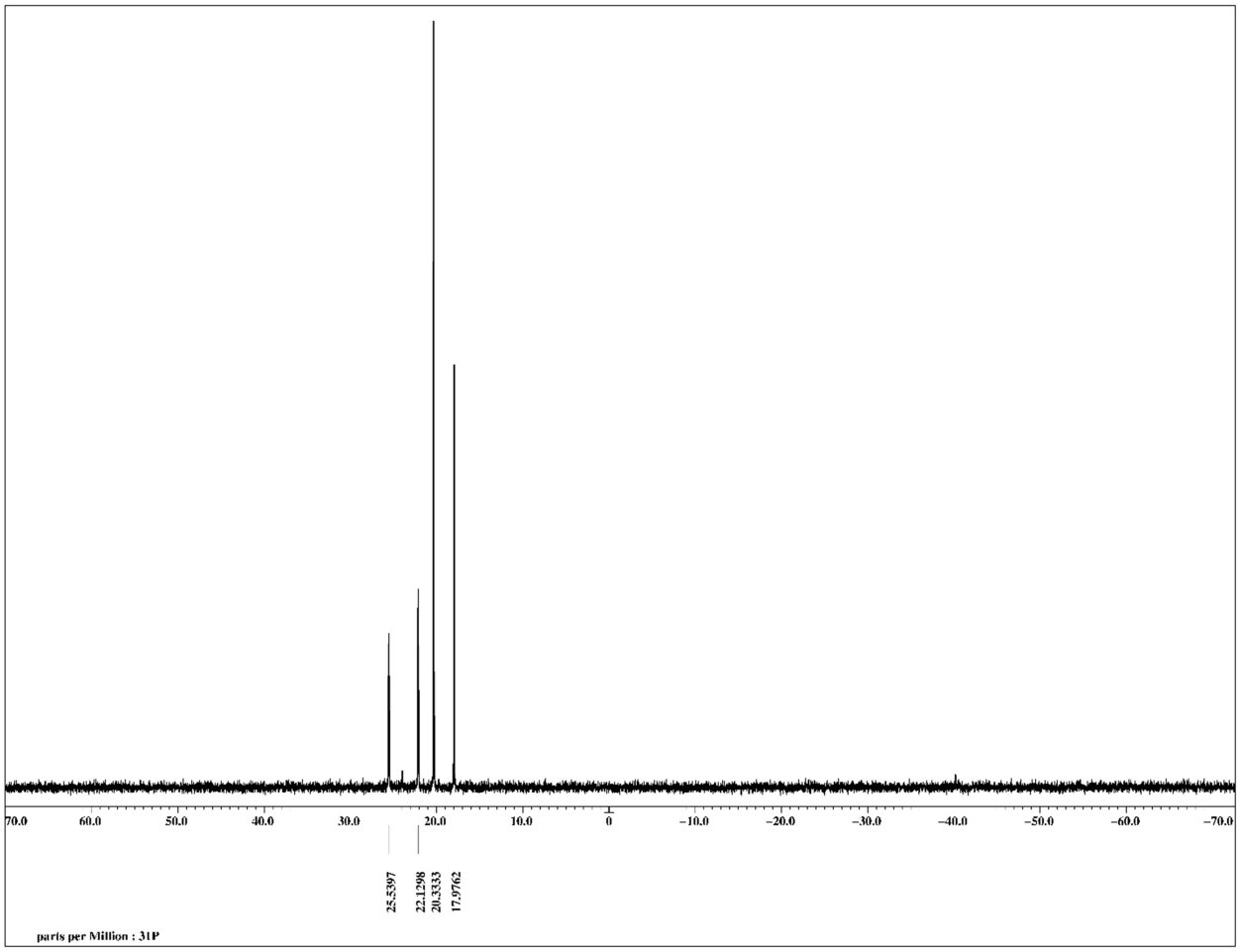

Figure S27. $^{31}P\{^{1}H\}$ NMR spectrum of Ph_2PBpin (1 eq) + 9-fluorenone-4-carbonyl chloride in C_6D_6.

Reactivity of Ph_2PBpin (2 equiv.) and 9-fluorenone-4-carbonyl chloride.

To a stirred toluene (2 mL) solution of 9-fluorenone-4-carbonyl chloride (75 mg, 0.31 mmol) was added a toluene (2 mL) solution of Ph_2PBpin (198 mg, 0.63 mmol). The reaction was allowed to proceed for 18 h at RT at which point the solvent was removed. Selected NMR data: ^1H NMR (400 MHz, C_6D_6) δ: 8.03 (m, Ar), 7.88 (dd, J = 7.8, 3.7 Hz, Ar), 7.53-7.42 (ov m, Ar), 7.34 (d, J = 7.3 Hz, Ar), 7.26 (m, Ar), 7.03 (m, Ar), 6.95-6.82 (ov m, Ar), 6.64 (t, J_{HH} = 7.8 Hz, Ar), 0.83 (s, ClBpin), 0.63 (s), 0.59 (s); ^{11}B NMR (128 MHz, C_6D_6) δ: 26.7 (sharp, ClBpin), 21 (br); $^{31}P\{^1H\}$ NMR (162 MHz, C_6D_6) δ: 82.3 (minor), 25.7 (minor), 24.0 (minor), 22.1 (major), 20.3 (minor), 18.0 (major), 17.2 (minor), -14.4 (minor, $Ph_2PPPh_2)PPh_2$).

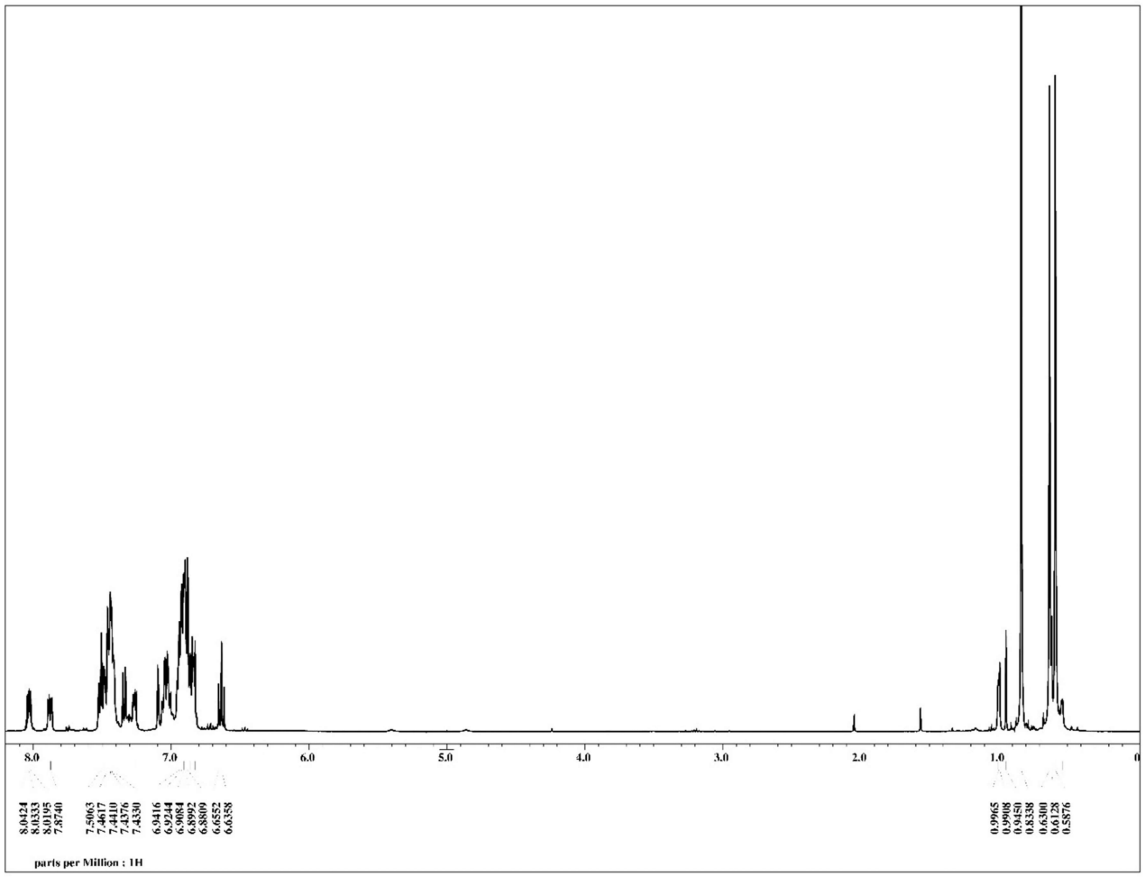

Figure S28. ^1H NMR spectrum of Ph_2PBpin (2 eq) + 9-fluorenone-4-carbonyl chloride in C_6D_6.

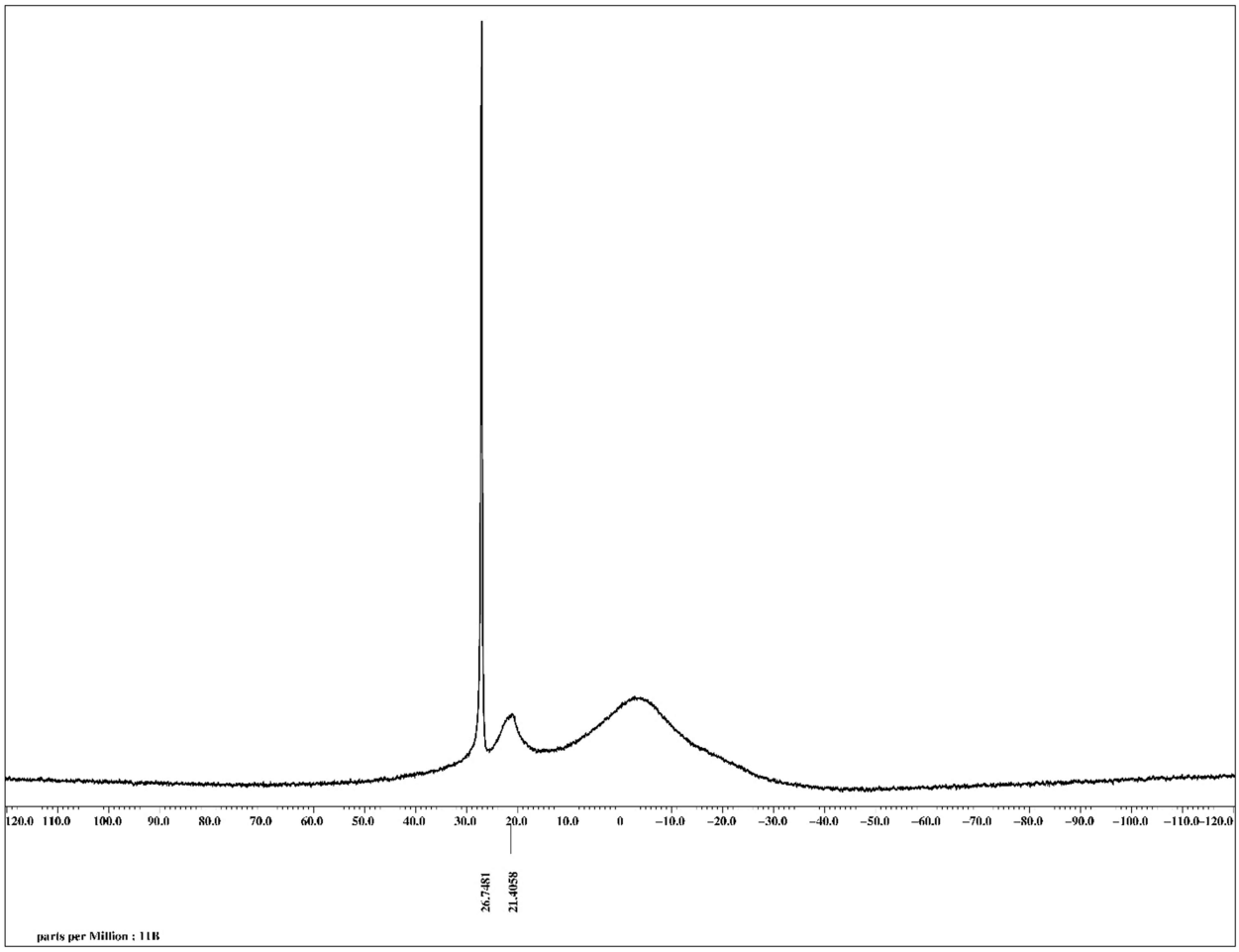

Figure S29. ^{11}B NMR spectrum of Ph_2PBpin (2 eq) + 9-fluorenone-4-carbonyl chloride in C_6D_6.

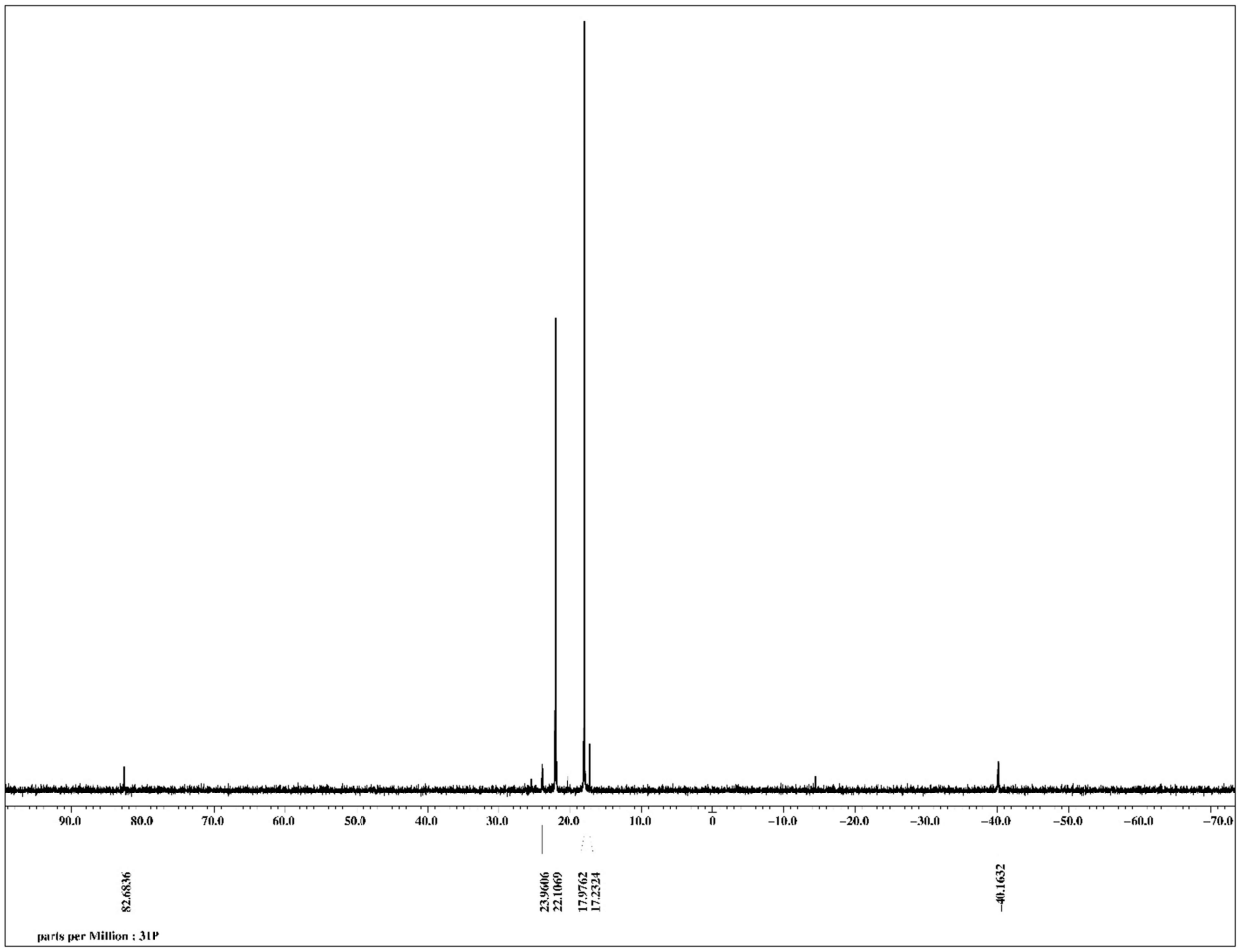

Figure S30. $^{31}P\{^{1}H\}$ NMR spectrum of Ph_2PBpin (2 eq) + 9-fluorenone-4-carbonyl chloride in C_6D_6.

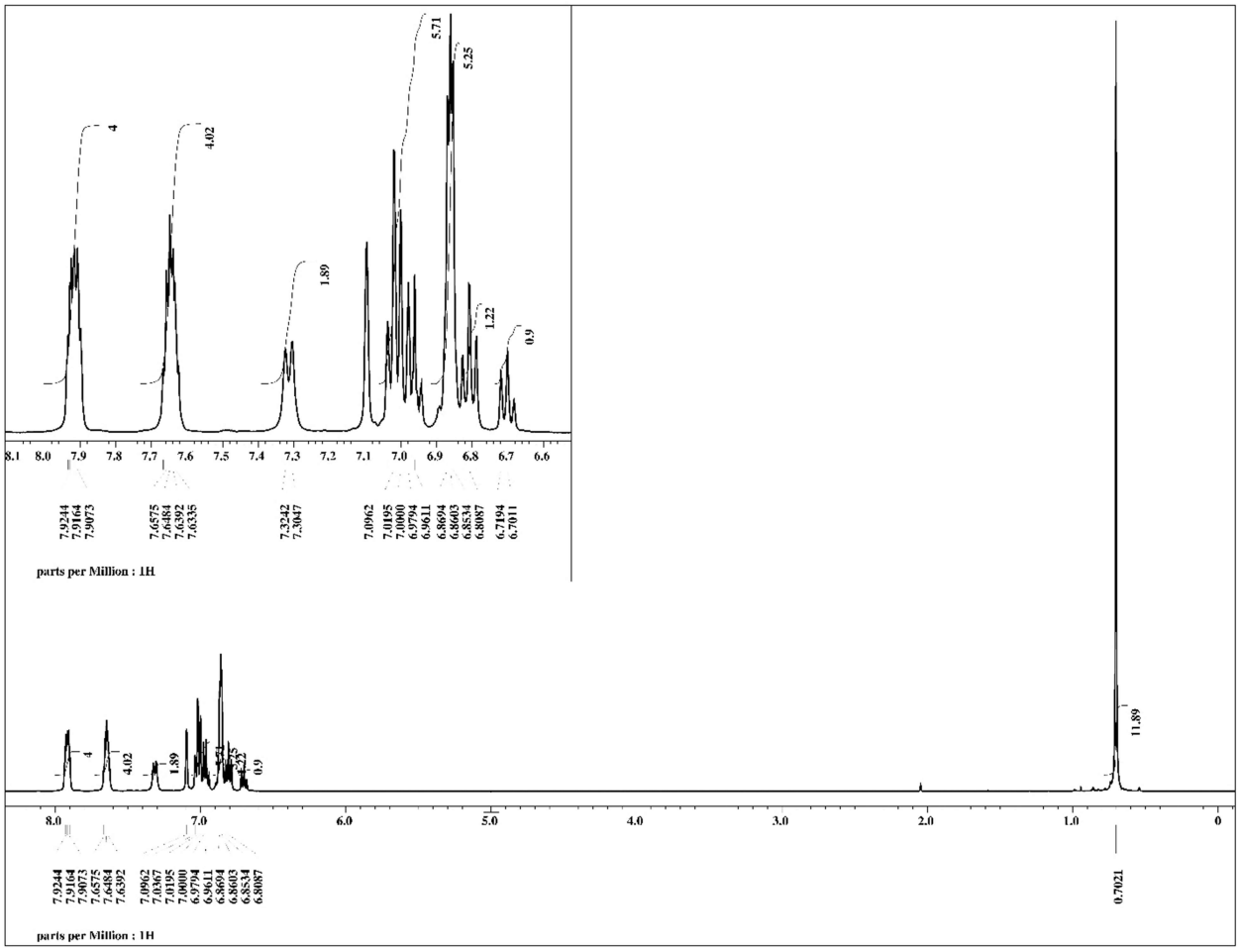

Figure S31. ^{1}H NMR spectrum of (phenyl((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)methylene)bis(diphenylphosphine), PhC(OBpin)(PPh_2)$_2$, **2a** in C_6D_6.

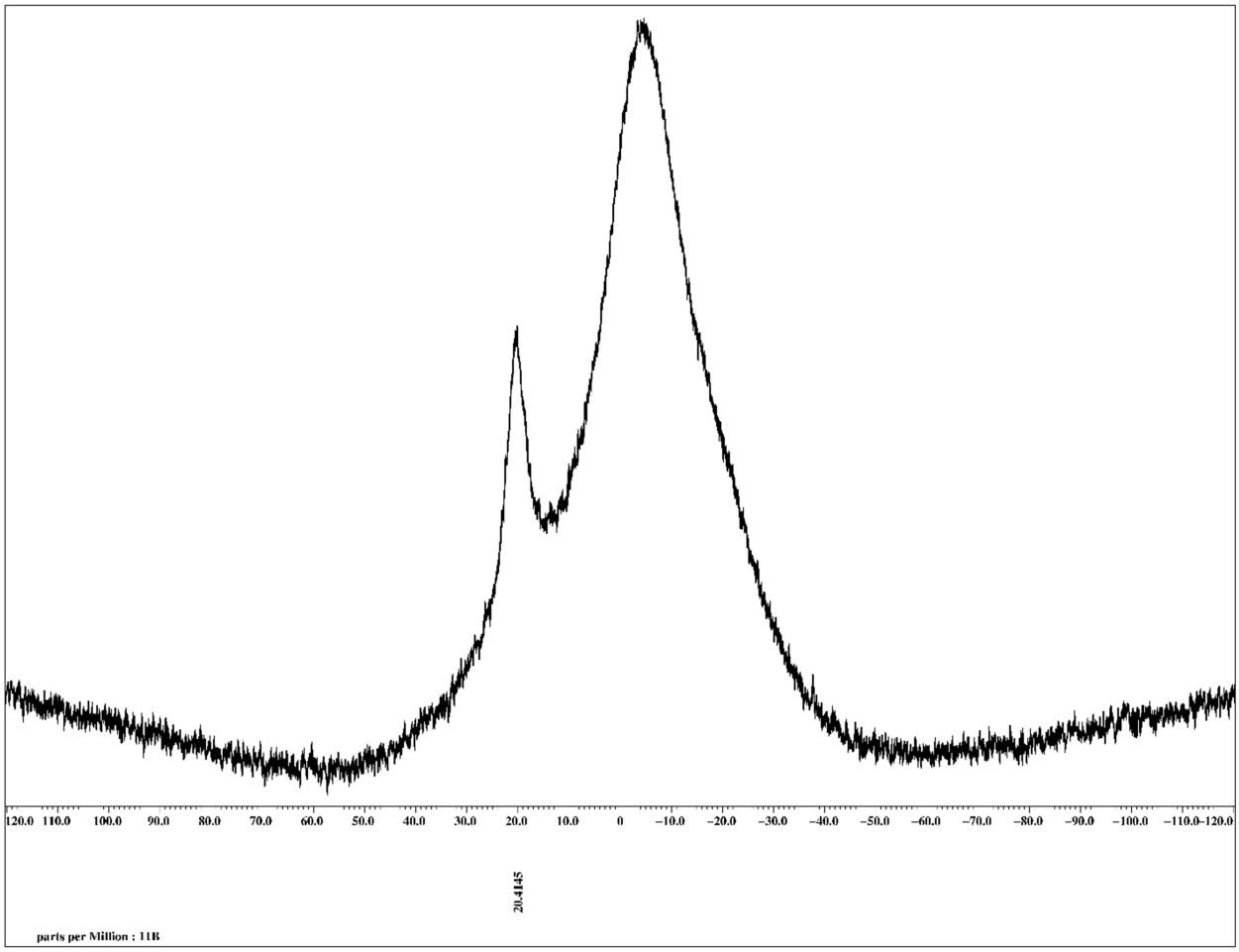

Figure S32. ^{11}B NMR spectrum of (phenyl((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)methylene)bis(diphenylphosphine), $PhC(OBpin)(PPh_2)_2$, **2a** in C_6D_6.

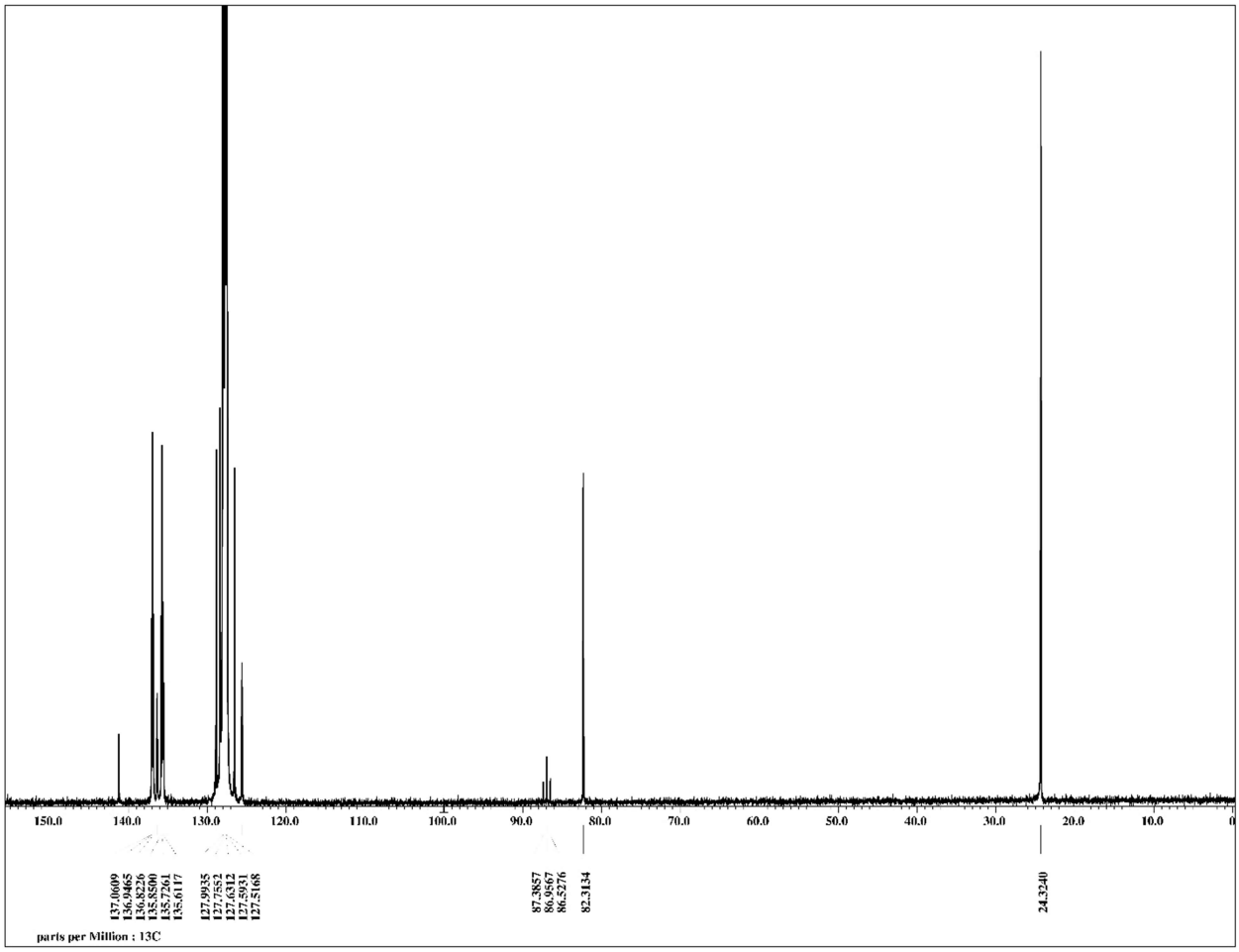

Figure S33. $^{13}C\{^{1}H\}$ NMR spectrum of (phenyl((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)methylene)bis(diphenylphosphine), $PhC(OBpin)(PPh_2)_2$, **2a** in C_6D_6.

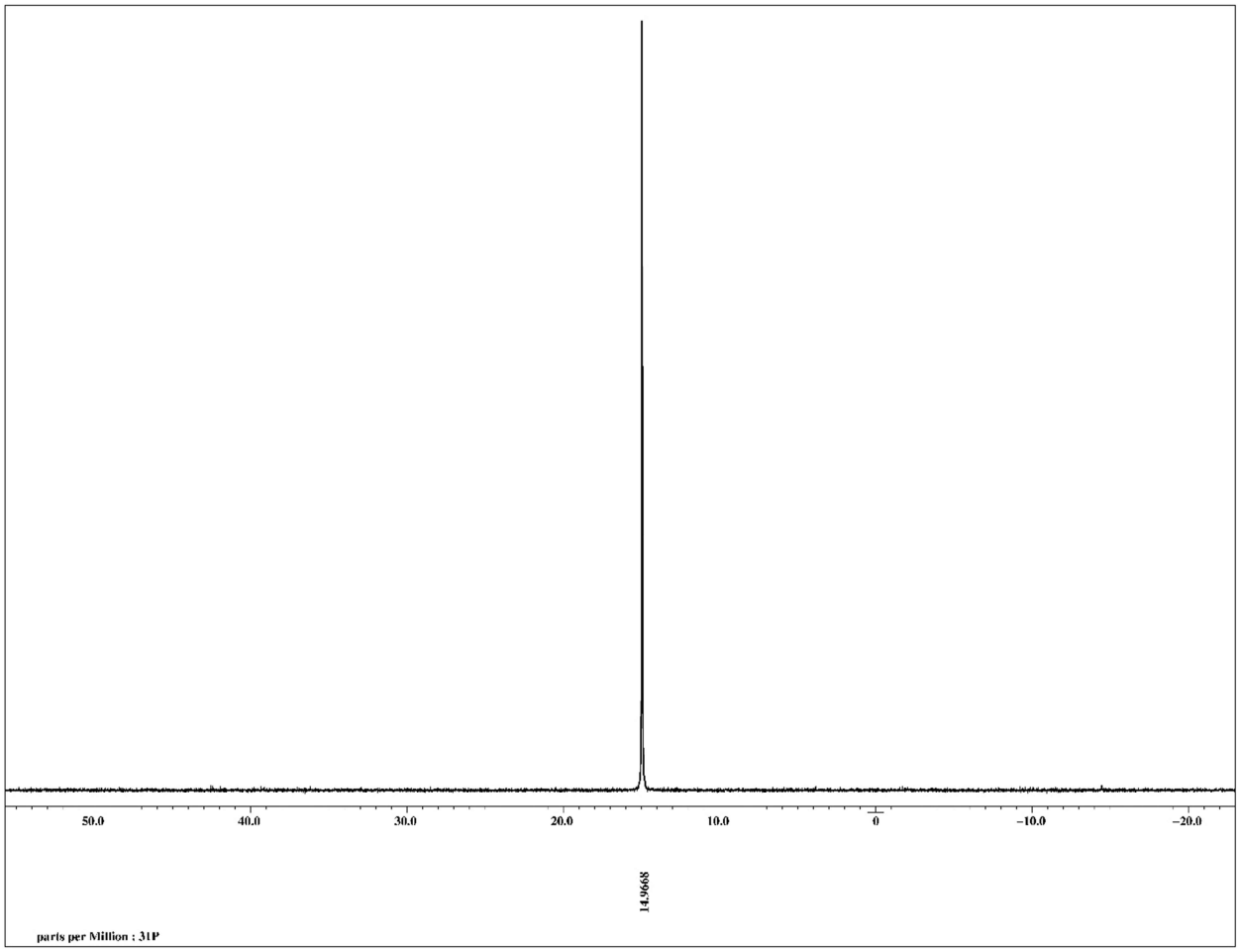

Figure S34. $^{31}P\{^{1}H\}$ NMR spectrum of (phenyl((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)methylene)bis(diphenylphosphine), $PhC(OBpin)(PPh_2)_2$, **2a** in C_6D_6.

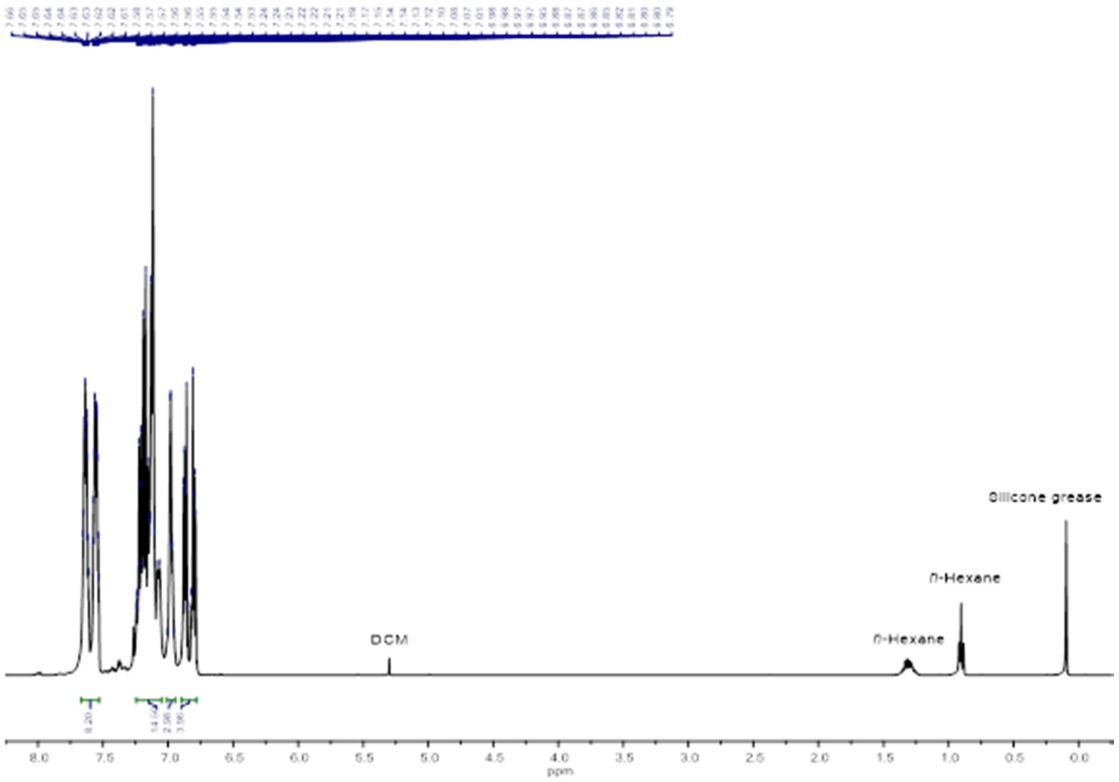

Figure S35. ^{1}H NMR spectrum of ((benzo[*d*][1,3,2]dioxaborol-2-yloxy)(phenyl)methylene)bis(diphenylphosphine), PhC(OBcat)(PPh_2)$_2$, **2b** in $CDCl_3$.

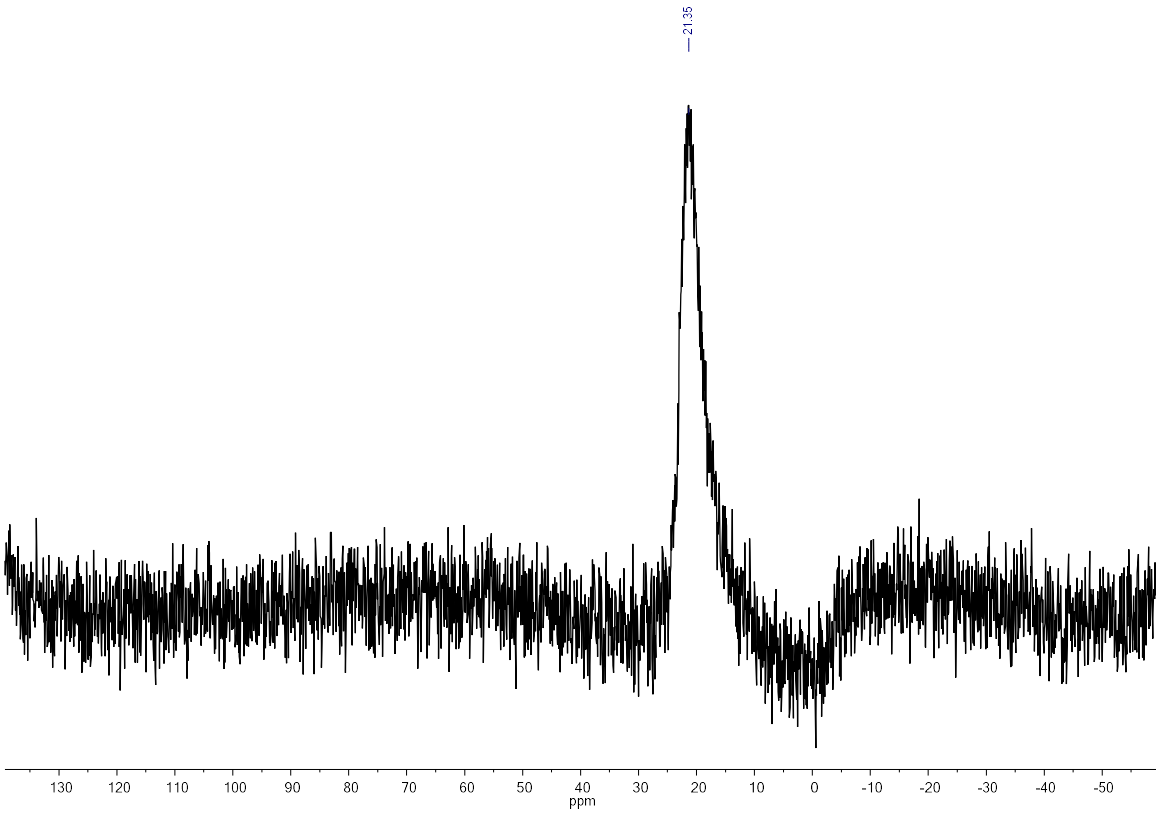

Figure S36. ^{11}B NMR spectrum of ((benzo[*d*][1,3,2]dioxaborol-2-yloxy)(phenyl)methylene)bis(diphenylphosphine), $PhC(OBcat)(PPh_2)_2$, **2b** in $CDCl_3$.

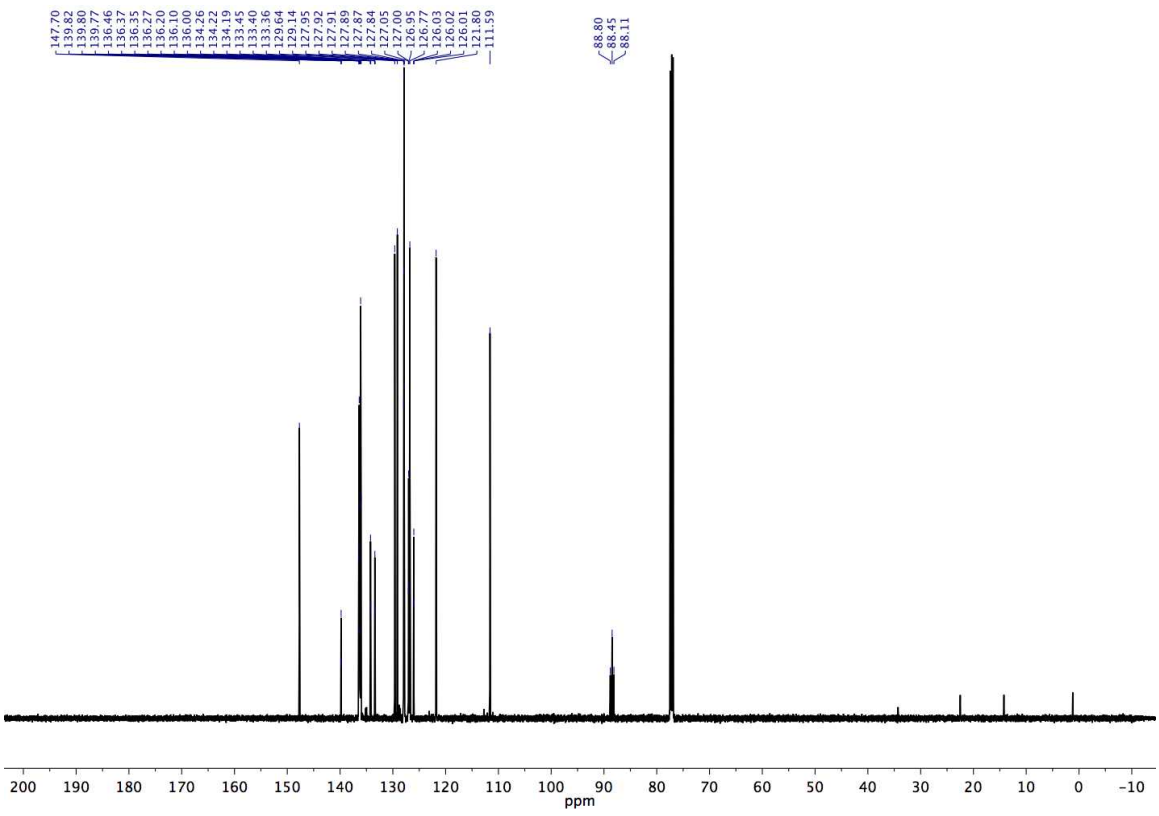

Figure S37. $^{13}C\{^{1}H\}$ NMR spectrum of ((benzo[*d*][1,3,2]dioxaborol-2-yloxy)(phenyl)methylene)bis(diphenylphosphine), $PhC(OBcat)(PPh_2)_2$, **2b** in $CDCl_3$.

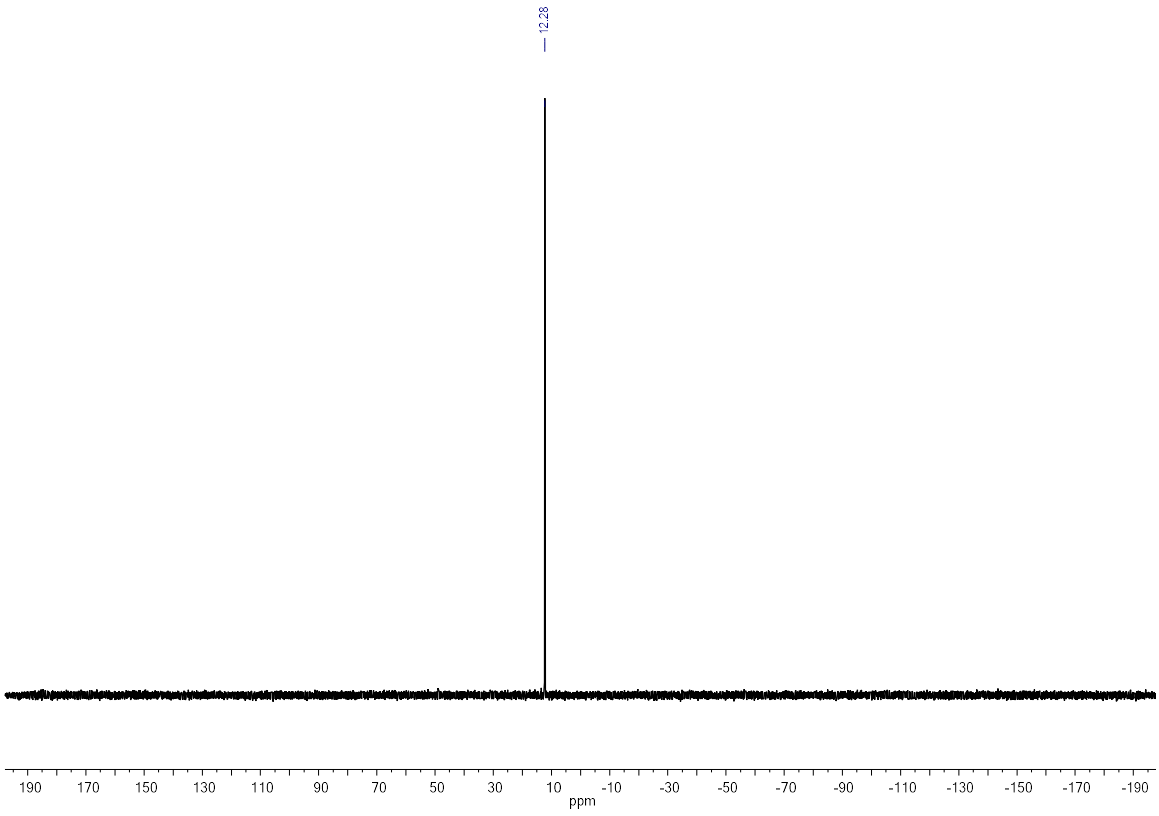

Figure S38. $^{31}P\{^{1}H\}$ NMR spectrum of ((benzo[*d*][1,3,2]dioxaborol-2-yloxy)(phenyl)methylene)bis(diphenylphosphine), $PhC(OBcat)(PPh_2)_2$, **2b** in $CDCl_3$.

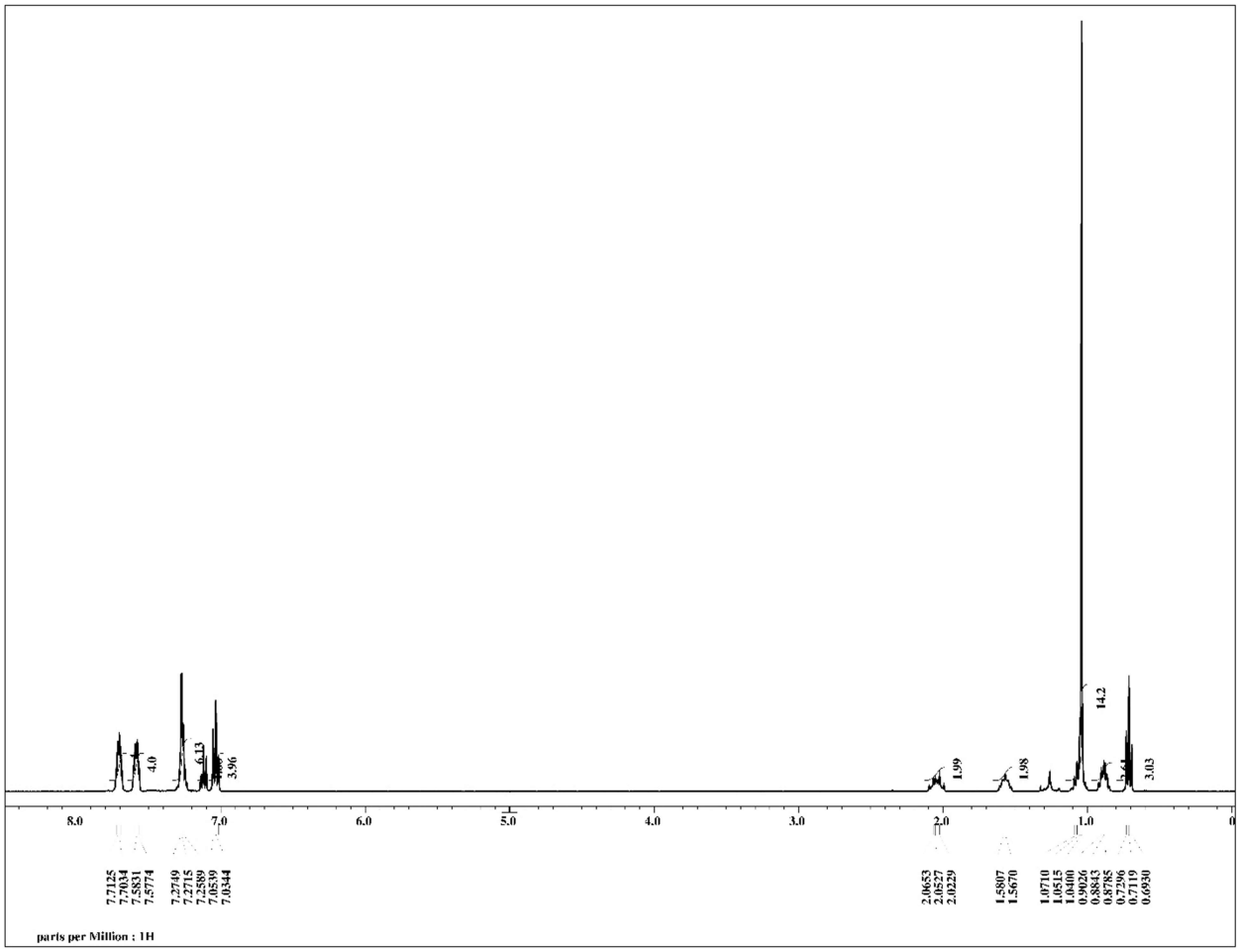

Figure S39. ^{1}H NMR spectrum of (1-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)hexane-1,1-diyl)bis(diphenylphosphine), *n*-pentylC(OBpin)(PPh_2)$_2$, **2d** in $CDCl_3$.

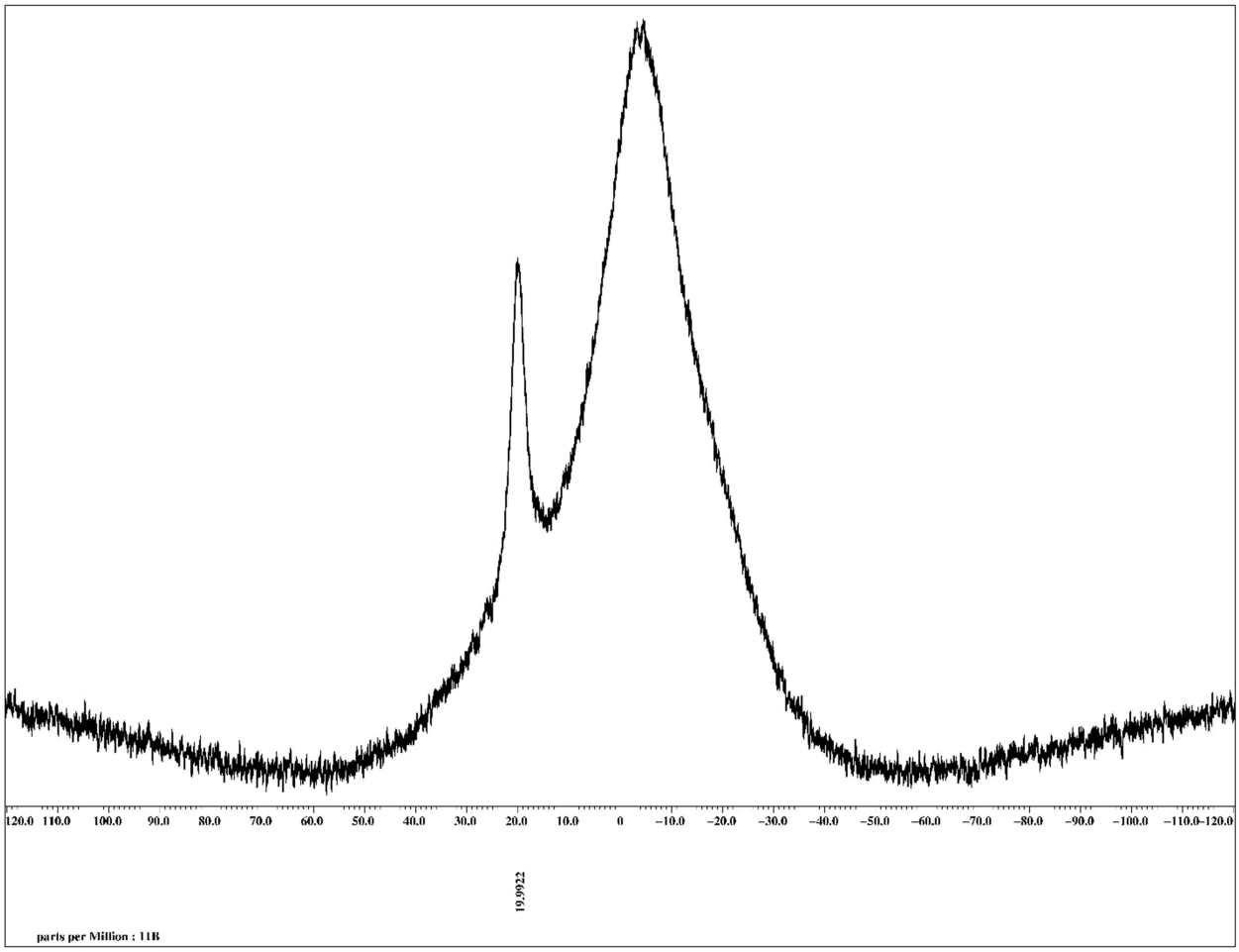

Figure S40. ^{11}B NMR spectrum of (1-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)hexane-1,1-diyl)bis(diphenylphosphine), *n*-pentylC(OBpin)$(PPh_2)_2$, **2d** in $CDCl_3$.

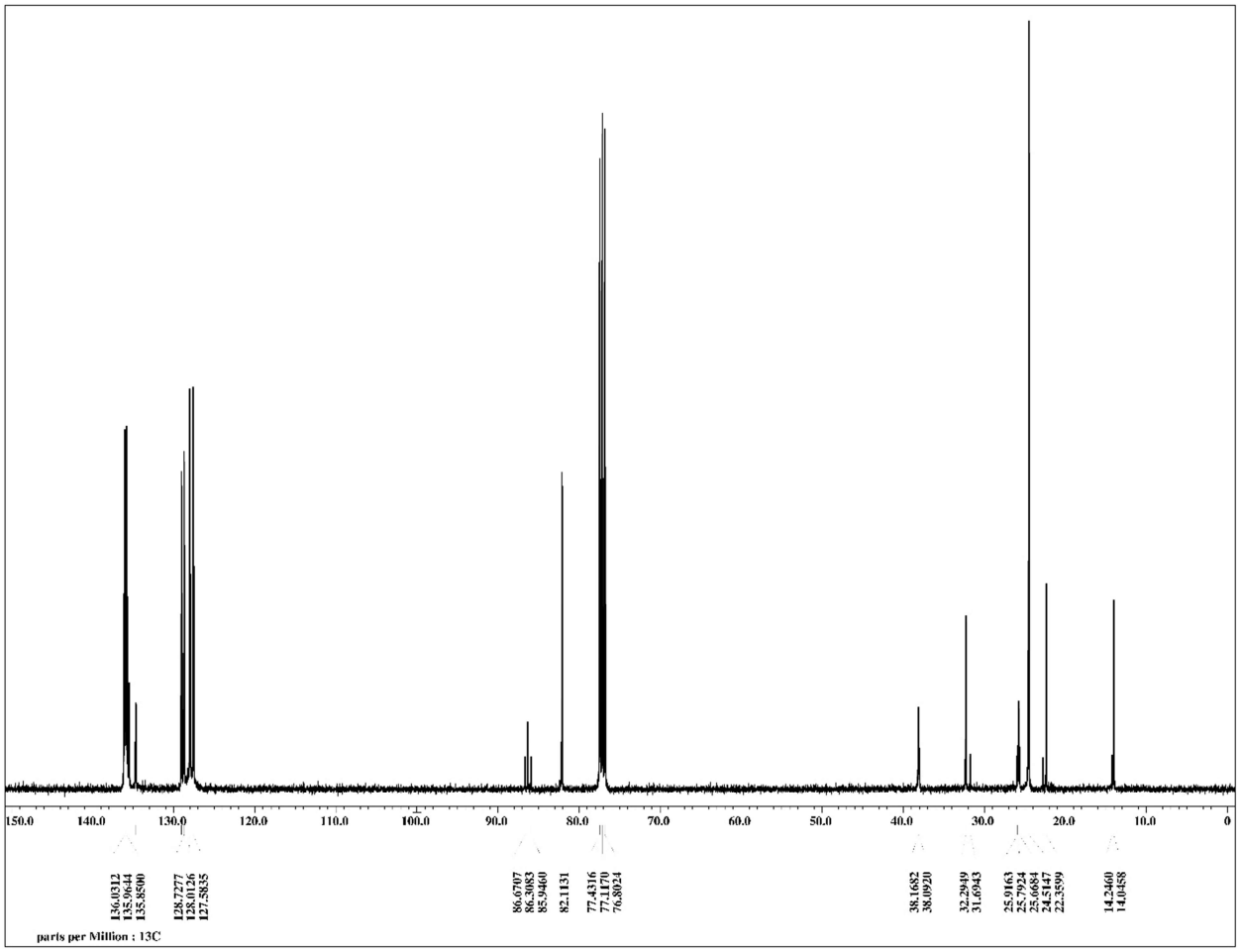

Figure S41. $^{13}C\{^{1}H\}$ NMR spectrum of (1-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)hexane-1,1-diyl)bis(diphenylphosphine), *n*-pentylC(OBpin)(PPh_2)$_2$, **2d** in $CDCl_3$.

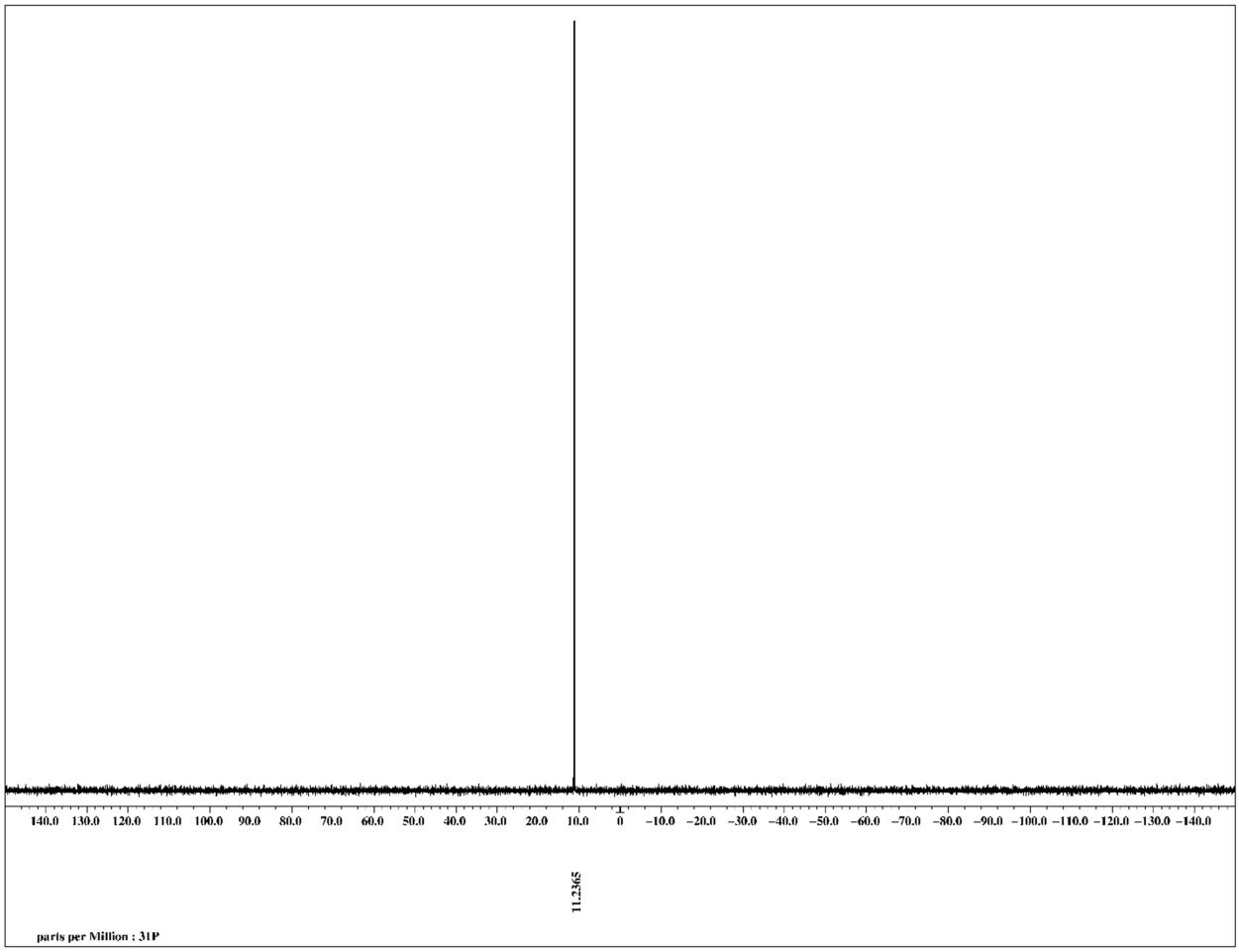

Figure S42. $^{31}P\{^{1}H\}$ NMR spectrum of (1-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)hexane-1,1-diyl)bis(diphenylphosphine), *n*-pentylC(OBpin)$(PPh_2)_2$, **2d** in $CDCl_3$.

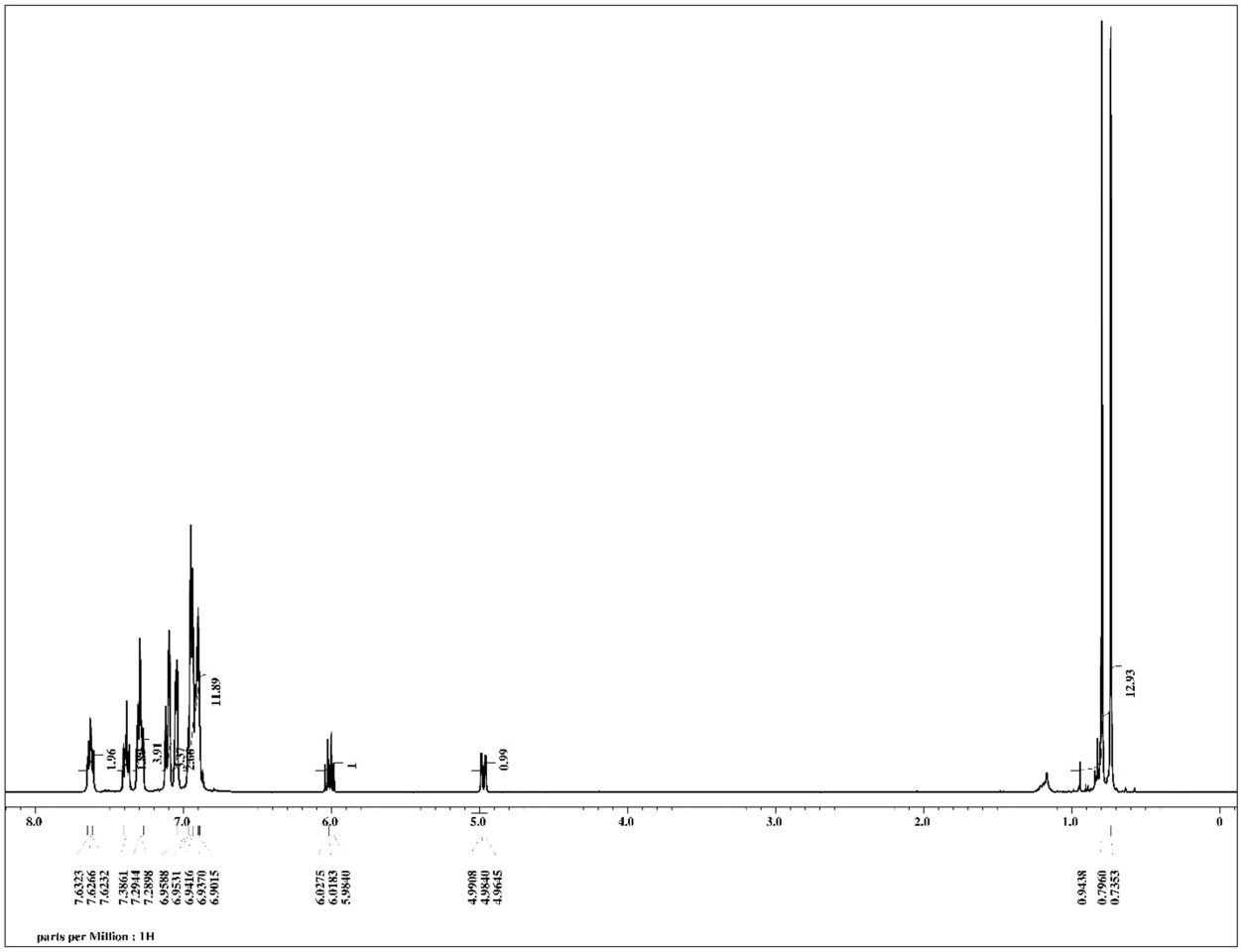

Figure S43. ^{1}H NMR spectrum of (*E*)-(3-phenyl-1-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)prop-1-ene-1,3-diyl)bis(diphenylphosphine), **2f** in C_6D_6.

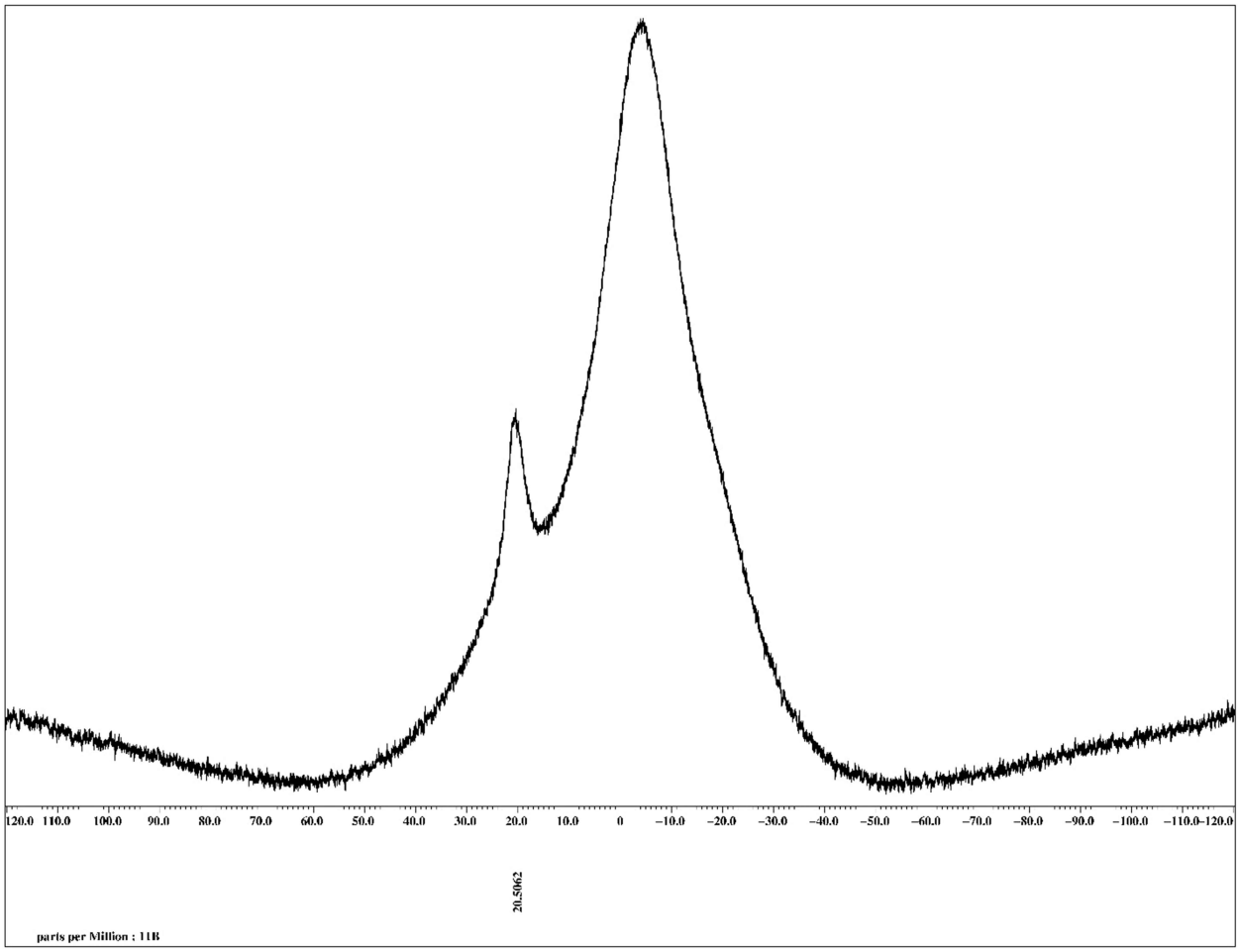

Figure S44. ^{11}B NMR spectrum of (*E*)-(3-phenyl-1-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)prop-1-ene-1,3-diyl)bis(diphenylphosphine), **2f** in C_6D_6.

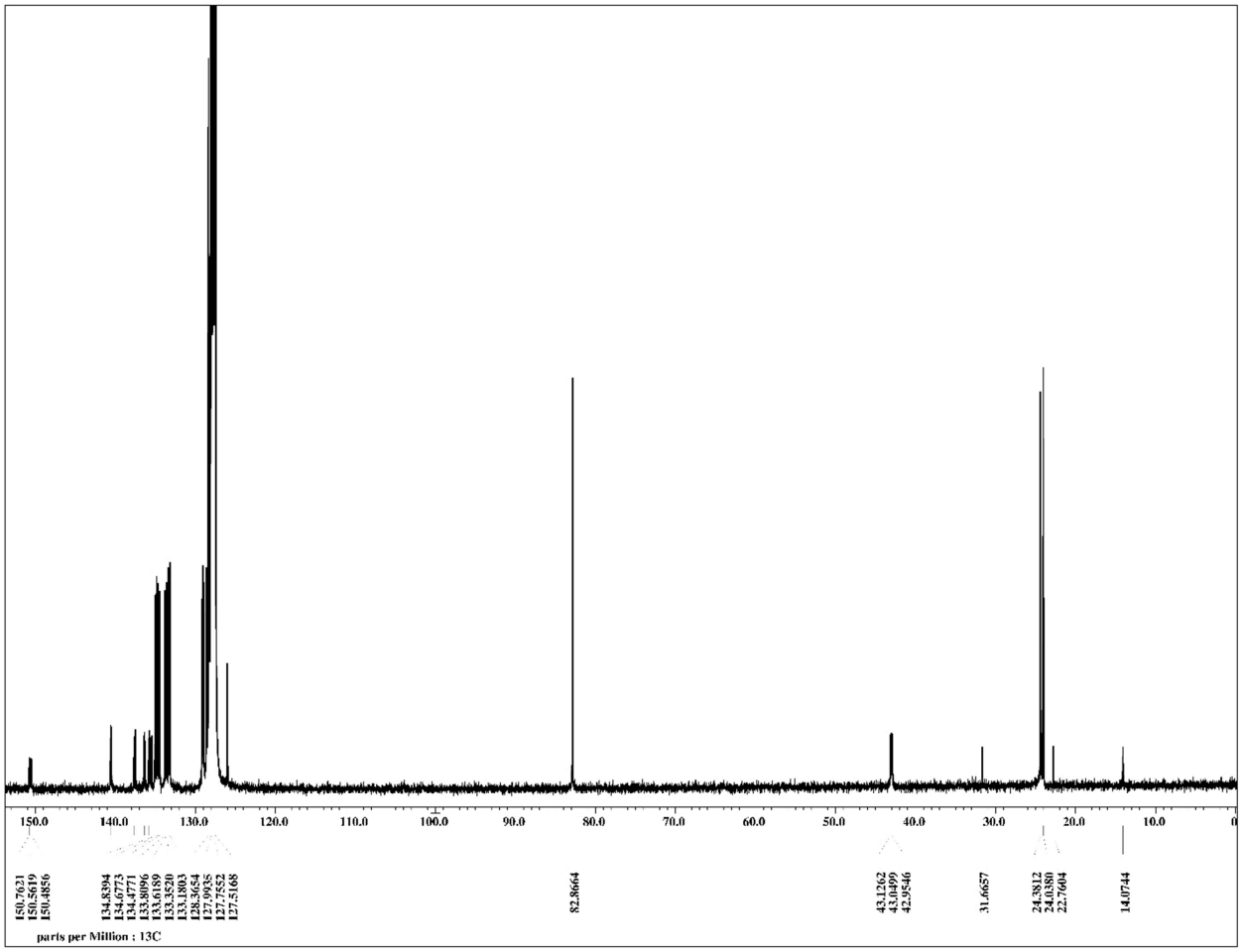

Figure S45. $^{13}C\{^{1}H\}$ NMR spectrum of (*E*)-(3-phenyl-1-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)prop-1-ene-1,3-diyl)bis(diphenylphosphine), **2f** in C_6D_6.

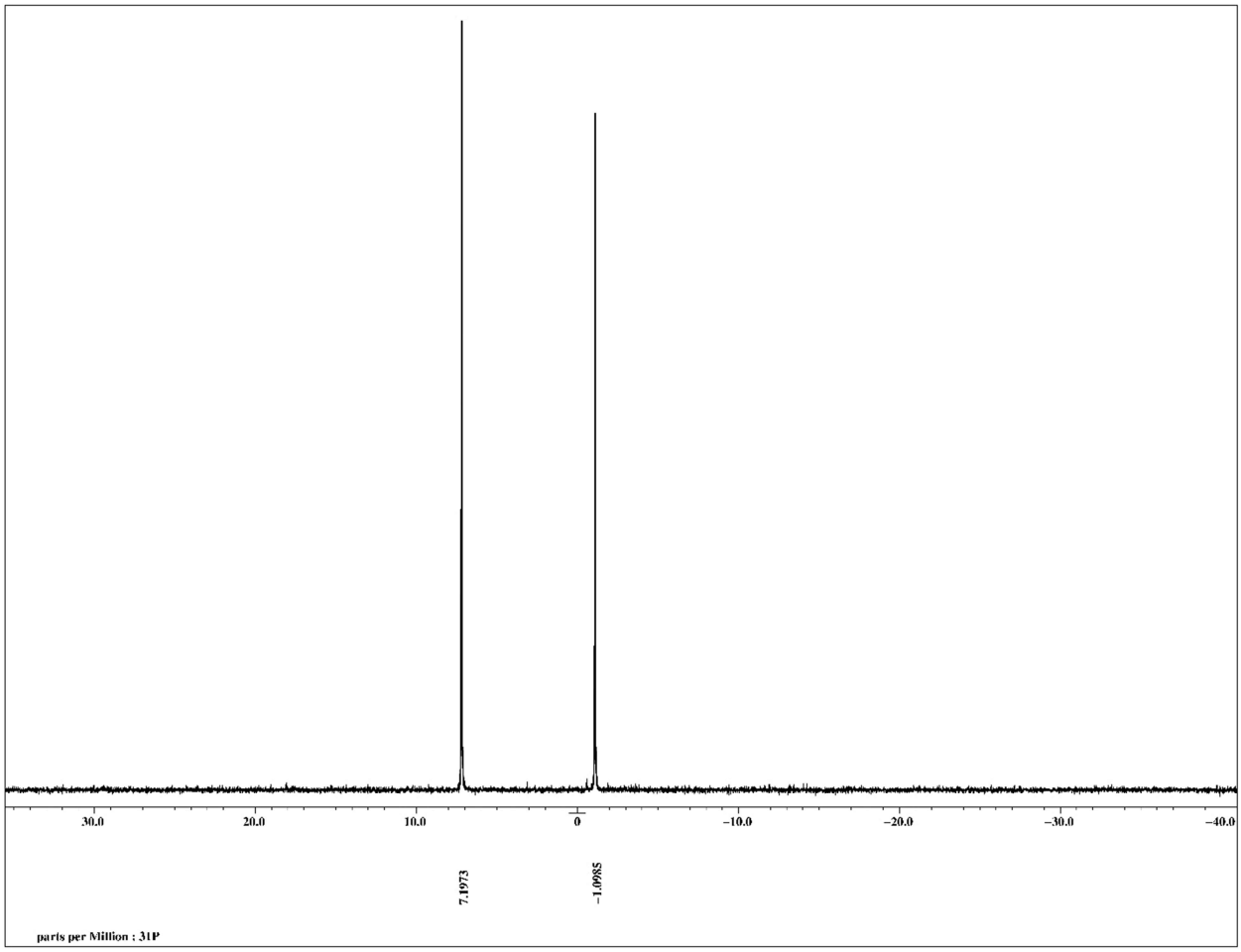

Figure S46. $^{31}P\{^{1}H\}$ NMR spectrum of (*E*)-(3-phenyl-1-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)prop-1-ene-1,3-diyl)bis(diphenylphosphine), **2f** in C_6D_6.

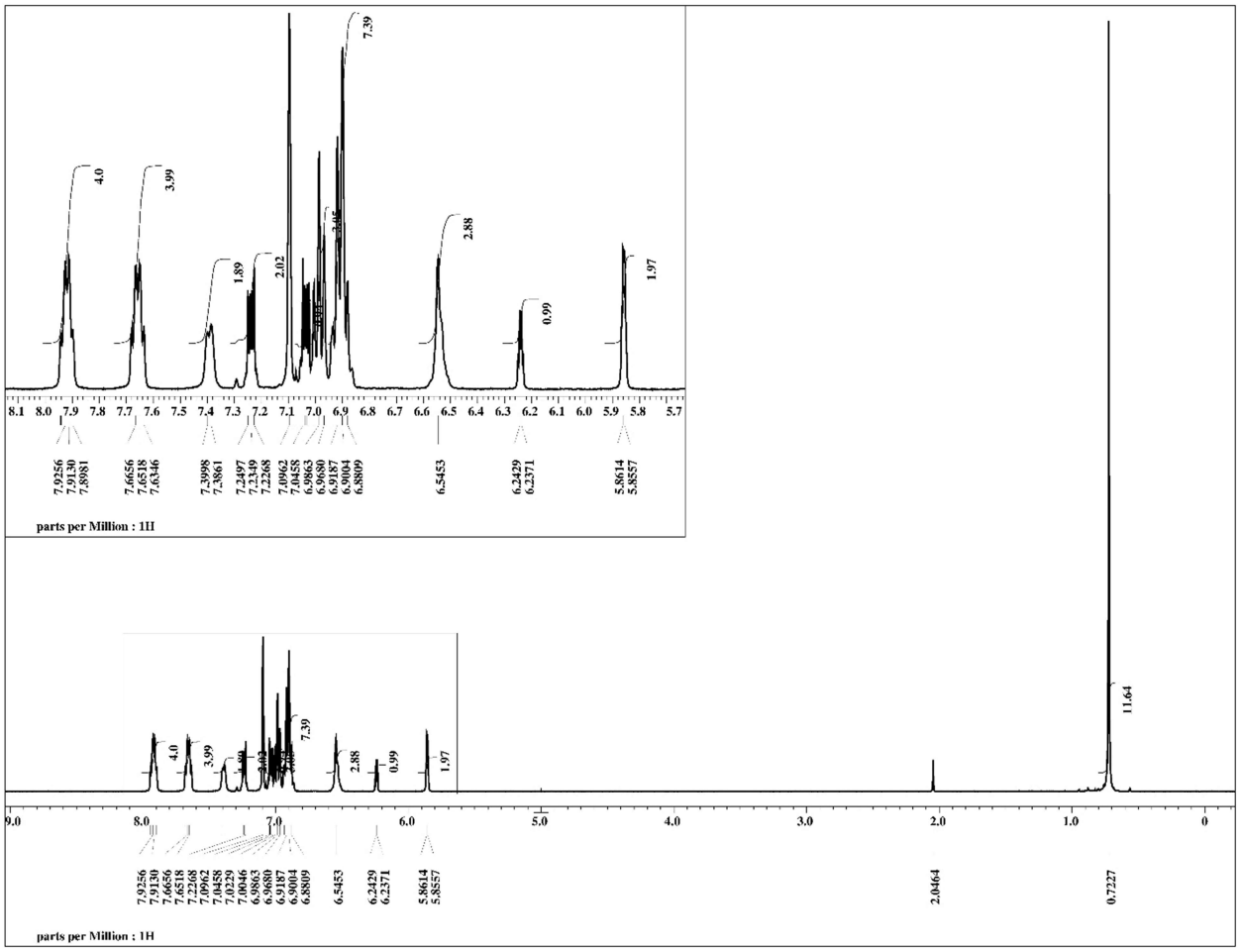

Figure S47. ^{1}H NMR spectrum of (η^5-C_9H_7)Rh(PhC(OBpin)(PPh_2)$_2$), **3a** in C_6D_6.

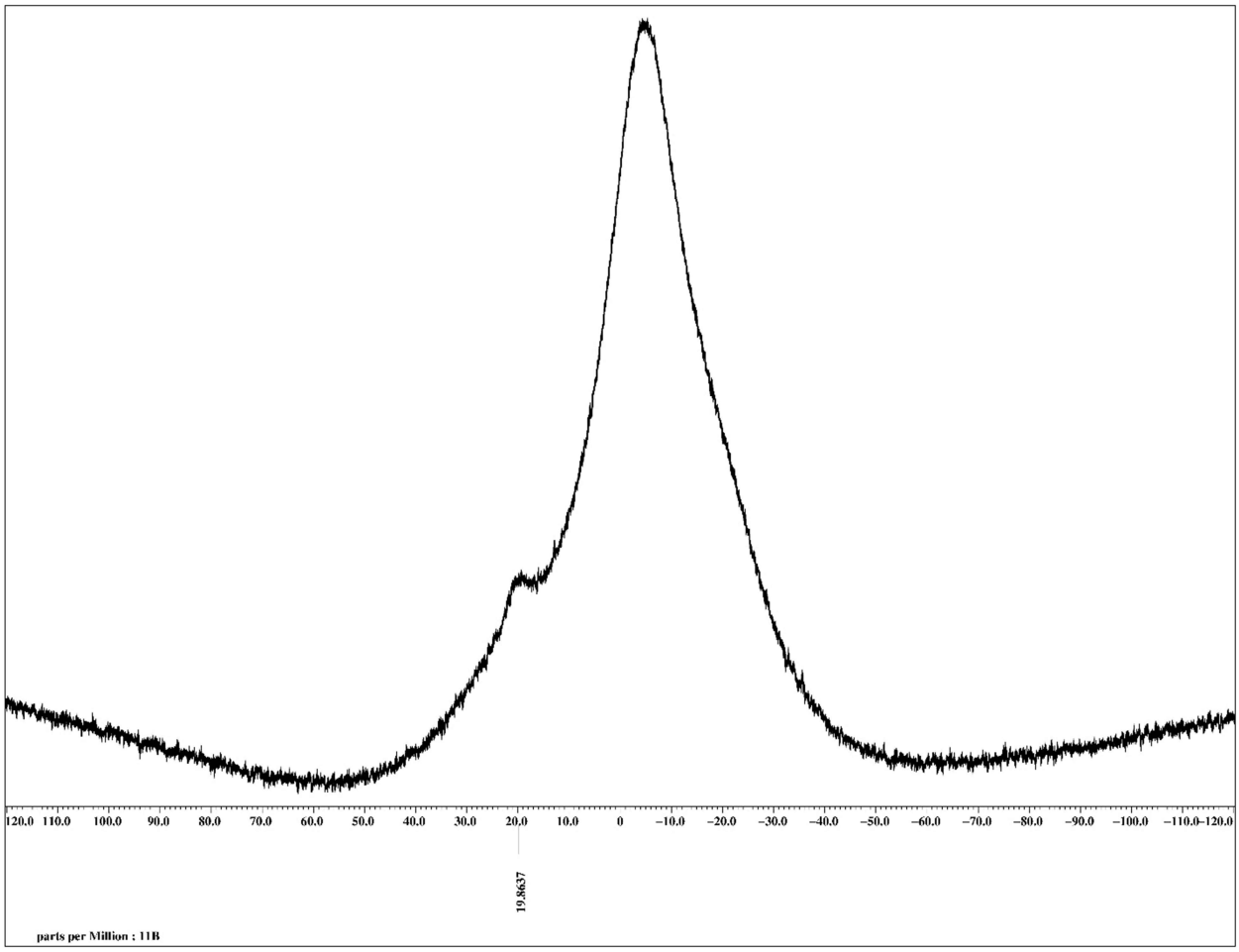

Figure S48. ^{11}B NMR spectrum of (η^5-C_9H_7)Rh(PhC(OBpin)(PPh_2)$_2$), **3a** in C_6D_6.

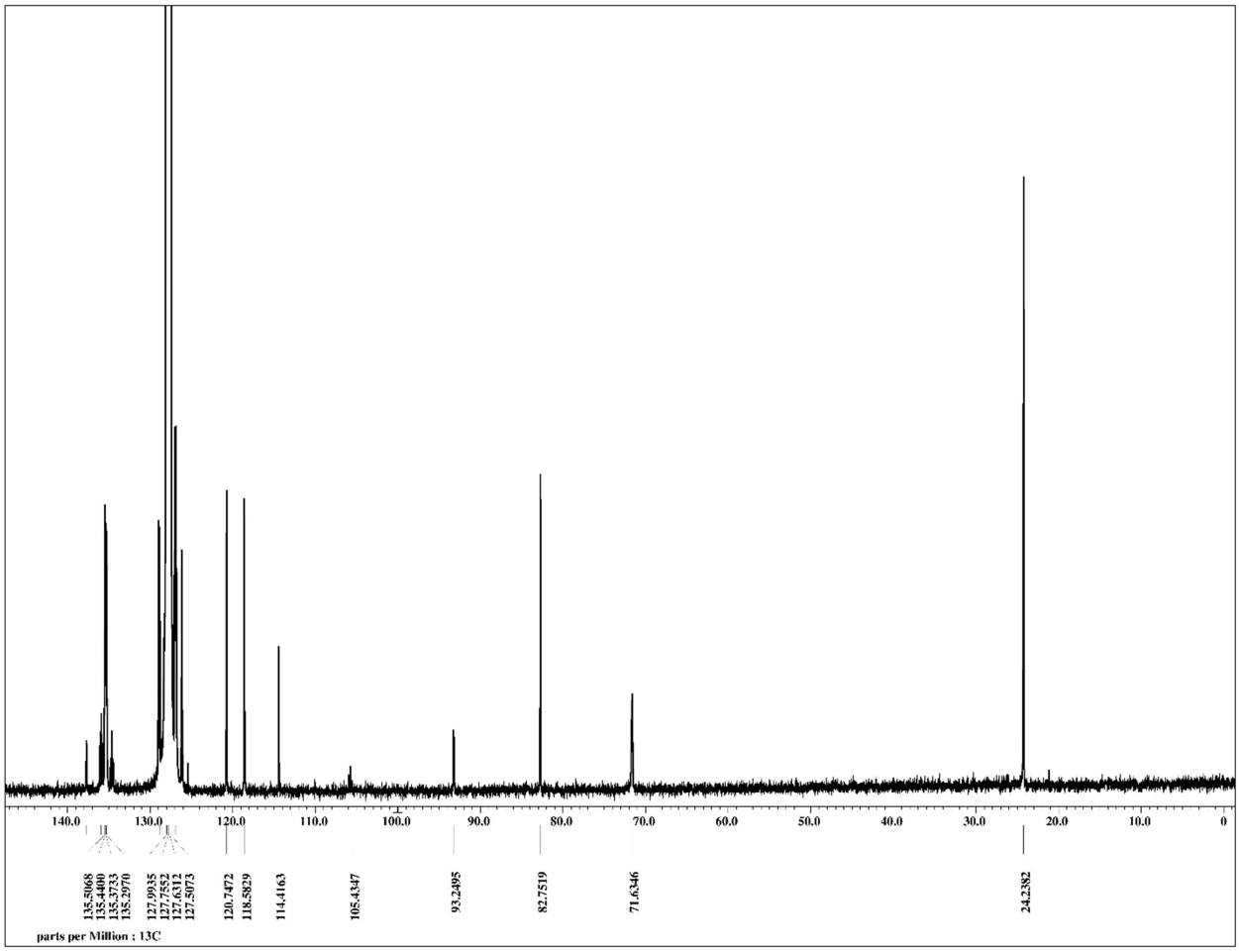

Figure S49. $^{13}C\{^{1}H\}$ NMR spectrum of (η^5-C_9H_7)Rh(PhC(OBpin)(PPh_2)$_2$), **3a** in C_6D_6.

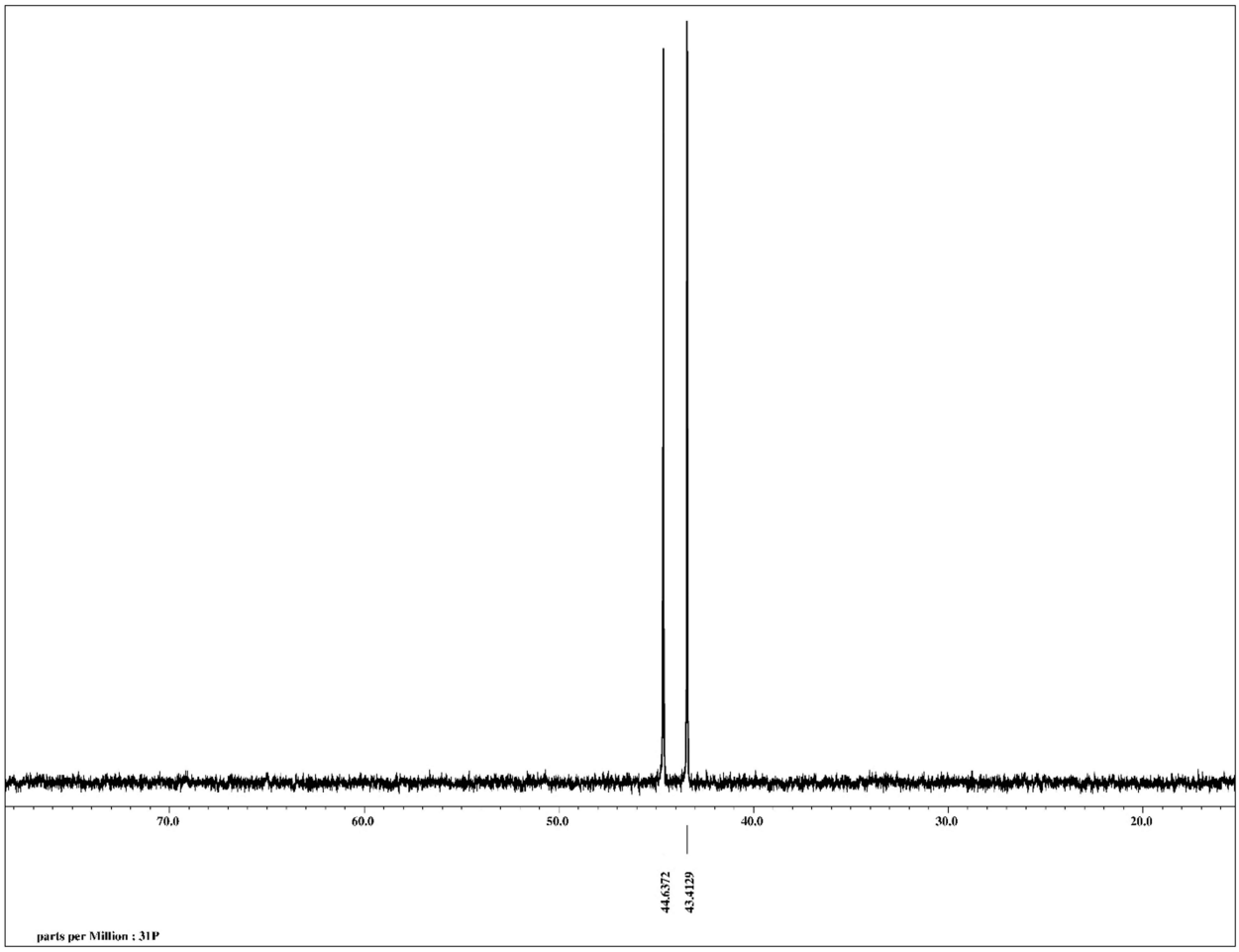

Figure S50. $^{31}P\{^{1}H\}$ NMR spectrum of (η^5-C_9H_7)Rh(PhC(OBpin)(PPh_2)$_2$), **3a** in C_6D_6.

Crystallography

Crystallographic data and structure refinement summary for 1b, 2b, and 2f.

Single crystals of **1b** and **2b** were grown from CH_2Cl_2 solutions layered with pentane while crystals of **2f** were grown from a saturated hexane solution. The crystals were coated with paratone oil, mounted on a cryoloop and frozen under a stream of cold nitrogen. Data were collected on a Bruker Apex2 X-ray diffractometer at 150 (2) K for all crystals using graphite monochromated Mo-Kα radiation (0.71073 Å). Data were collected using Bruker APEX-2 or APEX-3 software and processed using SHELX and an absorption correction applied using multi-scan within the APEX-2 or APEX-3 program. All structures were solved and refined by direct methods within the SHELXTL package.

Crystallographic data and structure refinement summary for 3a.

Crystals suitable for Xray crystallography of **3a** were grown from a saturated solution of toluene. Crystals for investigation were covered in paratone oil, mounted into a goniometer head, and then rapidly cooled under a stream of cold N_2 of the low-temperature apparatus (Oxford Cryostream) attached to the diffractometer. The data were then collected using the APEX3 software suite[1] on a Bruker Photon 100 CMOS diffractometer using a graphite monochromator with MoK_α (λ = 0.71073 Å) radiation. Data were collected at 170 K. APEX3 software was used for data reductions and SADABS[2] was used for absorption corrections (multi-scan; semi-empirical from equivalents). XPREP was used to determine the space group and the structures were solved and refined using the SHELX[3] software suite as implemented in the OLEX2[4] program suite.

Table 1. Crystallographic data-collection parameters for **1b**, **2b**, **2f**, and **3a**.

Complex	**1b**	**2b**	**2f**	**3a**
Formula	$C_{25}H_{27}OP$	$C_{37}H_{29}BO_3P_2$	$C_{39}H_{39}BO_3P_2$	$C_{46}H_{44}BO_3P_2Rh$
Molecular weight	374.43	594.35	628.45	820.47
Crystal system	Triclinic	Triclinic	Triclinic	Monoclinic
Space group	P-1	P-1	P-1	$P2_1$
a/Å	8.317(3)	10.299(4)	12.1297(6)	10.3384(5)
b/Å	11.854(4)	10.930(3)	12.7797(5)	17.0645(8)
c/Å	11.878(3)	14.818(5)	24.5958(11)	11.1586(6)
α/°	99.213(7)	76.664(12)	100.177(3)	90
β/°	105.491(8)	84.069(12)	90.169(4)	91.508(2)
γ/°	107.793(7)	68.725(12)	111.086(3)	90
V/Å^3	1036.7(5)	1512.2(9)	3492.2(3)	1967.91(17)
Z	2	2	4	2
ρ_{calc}/Mg m^{-3}	1.200	1.305	1.195	1.305
Crystal size/mm^3	0.070×0.060×0.050	0.090×0.070×0.050	0.120×0.100×0.090	0.36×0.142×0.065
Temp/K	150(2)	150(2)	150(2)	170.0
Radiation	Mo-K_α (λ=0.71073 Å)	Mo-K_α (λ=0.71073 Å)	Mo-K_α (λ=0.71073 Å)	Mo-K_α (λ=0.71073 Å)
μ/mm^{-1}	0.144	0.181	0.160	0.556
Total reflections	28397	43828	52892	96896
Total unique reflections	5148	7482	17312	10161
No. of variables	250	388	819	482
θ Range/°	2.734 to 28.306	1.413 to 28.285	1.687 to 28.291	2.972 to 28.788
Largest difference peak/hole/e Å^{-3}	0.290 and -0.298	0.288 and -0.314	0.554 and -0.431	0.27 and -0.33
S (GoF) on F^2	1.013	1.010	1.060	1.093
$R1^a$ ($I>2\sigma(I)$)	0.0491	0.0469	0.0516	0.0245
$wR2^b$ (all data)	0.1077	0.0969	0.1630	0.0498

[a]) $R1 = \sum||F_o|-|F_c||/\sum|F_o|$. [b]) $wR2 = (\sum[w(F_o^2-F_c^2)^2]/\sum[wF_o^4])^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (0.0371 \cdot P)^2 + (0.3604 \cdot P)]$ (**1b**), $1/[\sigma^2(F_o^2) + (0.0419 \cdot P)^2 + (0.7124 \cdot P)]$ (**2b**), $1/[\sigma^2(F_o^2) + (0.0792 \cdot P)^2]$ (**2f**), and $1/[\sigma^2(F_o^2) + (0.0159 \cdot P)^2 + (0.8002 \cdot P)]$ (**3a**).

Table 2. Atomic coordinates (Åx10^4) and equivalent isotropic displacement parameters (Å^{2}x10^3)for **1b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	4549(1)	6969(1)	2636(1)	20(1)
O(1)	7194(2)	9171(1)	3551(1)	32(1)
C(1)	7094(2)	8100(2)	5069(2)	21(1)
C(2)	8608(2)	9036(2)	5921(2)	26(1)
C(3)	9350(3)	8888(2)	7051(2)	33(1)
C(4)	8582(3)	7810(2)	7342(2)	35(1)
C(5)	7074(3)	6881(2)	6506(2)	32(1)
C(6)	6327(3)	7024(2)	5376(2)	25(1)
C(7)	6382(2)	8282(2)	3838(2)	22(1)
C(8)	2431(2)	6506(2)	2942(2)	19(1)
C(9)	2009(2)	7128(2)	3876(2)	21(1)
C(10)	387(3)	6551(2)	4046(2)	26(1)
C(11)	-840(3)	5412(2)	3323(2)	26(1)
C(12)	-435(3)	4842(2)	2376(2)	26(1)
C(13)	1177(2)	5360(2)	2181(2)	20(1)
C(14)	3193(3)	8385(2)	4700(2)	28(1)
C(15)	-2575(3)	4815(2)	3537(2)	39(1)
C(16)	1528(3)	4673(2)	1140(2)	24(1)
C(17)	4316(2)	7579(2)	1300(2)	20(1)
C(18)	5447(3)	7391(2)	648(2)	26(1)
C(19)	5340(3)	7768(2)	-414(2)	29(1)
C(20)	4149(3)	8319(2)	-860(2)	27(1)
C(21)	3083(3)	8524(2)	-191(2)	25(1)
C(22)	3135(2)	8174(2)	881(2)	22(1)
C(23)	6806(3)	6807(2)	1077(2)	40(1)
C(24)	3993(3)	8673(2)	-2042(2)	37(1)
C(25)	1969(3)	8498(2)	1553(2)	33(1)

Table 3. Bond lengths [Å] and angles [°] for **1b**.

P(1)-C(8)	1.8306(19)
P(1)-C(17)	1.8356(18)
P(1)-C(7)	1.860(2)
O(1)-C(7)	1.219(2)
C(1)-C(6)	1.394(3)
C(1)-C(2)	1.395(3)
C(1)-C(7)	1.500(2)
C(2)-C(3)	1.383(3)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.386(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.383(3)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.381(3)
C(5)-H(5A)	0.9500
C(6)-H(6A)	0.9500
C(8)-C(13)	1.410(3)
C(8)-C(9)	1.415(2)
C(9)-C(10)	1.398(3)
C(9)-C(14)	1.506(3)
C(10)-C(11)	1.386(3)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.391(3)
C(11)-C(15)	1.509(3)
C(12)-C(13)	1.391(3)
C(12)-H(12A)	0.9500
C(13)-C(16)	1.513(3)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800

C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(22)	1.408(3)
C(17)-C(18)	1.413(3)
C(18)-C(19)	1.395(3)
C(18)-C(23)	1.516(3)
C(19)-C(20)	1.384(3)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.387(3)
C(20)-C(24)	1.512(3)
C(21)-C(22)	1.395(2)
C(21)-H(21A)	0.9500
C(22)-C(25)	1.506(3)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800

C(8)-P(1)-C(17)	110.68(8)
C(8)-P(1)-C(7)	113.72(8)
C(17)-P(1)-C(7)	102.35(9)
C(6)-C(1)-C(2)	119.27(17)
C(6)-C(1)-C(7)	122.44(17)
C(2)-C(1)-C(7)	118.27(16)
C(3)-C(2)-C(1)	120.22(18)
C(3)-C(2)-H(2A)	119.9
C(1)-C(2)-H(2A)	119.9
C(2)-C(3)-C(4)	119.92(19)
C(2)-C(3)-H(3A)	120.0
C(4)-C(3)-H(3A)	120.0
C(5)-C(4)-C(3)	120.25(19)

C(5)-C(4)-H(4A)	119.9
C(3)-C(4)-H(4A)	119.9
C(6)-C(5)-C(4)	120.06(19)
C(6)-C(5)-H(5A)	120.0
C(4)-C(5)-H(5A)	120.0
C(5)-C(6)-C(1)	120.28(18)
C(5)-C(6)-H(6A)	119.9
C(1)-C(6)-H(6A)	119.9
O(1)-C(7)-C(1)	120.91(17)
O(1)-C(7)-P(1)	118.94(14)
C(1)-C(7)-P(1)	118.63(13)
C(13)-C(8)-C(9)	119.35(16)
C(13)-C(8)-P(1)	113.36(13)
C(9)-C(8)-P(1)	127.17(14)
C(10)-C(9)-C(8)	118.37(17)
C(10)-C(9)-C(14)	117.46(17)
C(8)-C(9)-C(14)	124.17(17)
C(11)-C(10)-C(9)	122.90(18)
C(11)-C(10)-H(10A)	118.6
C(9)-C(10)-H(10A)	118.6
C(10)-C(11)-C(12)	117.76(18)
C(10)-C(11)-C(15)	121.41(19)
C(12)-C(11)-C(15)	120.82(19)
C(11)-C(12)-C(13)	121.82(18)
C(11)-C(12)-H(12A)	119.1
C(13)-C(12)-H(12A)	119.1
C(12)-C(13)-C(8)	119.70(17)
C(12)-C(13)-C(16)	118.61(17)
C(8)-C(13)-C(16)	121.68(16)
C(9)-C(14)-H(14A)	109.5
C(9)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(9)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(11)-C(15)-H(15A)	109.5

C(11)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(11)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(22)-C(17)-C(18)	119.34(16)
C(22)-C(17)-P(1)	126.64(14)
C(18)-C(17)-P(1)	114.01(14)
C(19)-C(18)-C(17)	119.38(18)
C(19)-C(18)-C(23)	118.52(17)
C(17)-C(18)-C(23)	122.09(16)
C(20)-C(19)-C(18)	122.13(18)
C(20)-C(19)-H(19A)	118.9
C(18)-C(19)-H(19A)	118.9
C(19)-C(20)-C(21)	117.54(17)
C(19)-C(20)-C(24)	121.46(19)
C(21)-C(20)-C(24)	121.00(19)
C(20)-C(21)-C(22)	123.01(18)
C(20)-C(21)-H(21A)	118.5
C(22)-C(21)-H(21A)	118.5
C(21)-C(22)-C(17)	118.56(17)
C(21)-C(22)-C(25)	117.87(17)
C(17)-C(22)-C(25)	123.53(16)
C(18)-C(23)-H(23A)	109.5
C(18)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(18)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(20)-C(24)-H(24A)	109.5

C(20)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(20)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(22)-C(25)-H(25A)	109.5
C(22)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(22)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for **1b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	18(1)	25(1)	17(1)	7(1)	6(1)	8(1)
O(1)	33(1)	30(1)	26(1)	12(1)	7(1)	1(1)
C(1)	18(1)	28(1)	18(1)	6(1)	6(1)	10(1)
C(2)	22(1)	28(1)	25(1)	9(1)	7(1)	6(1)
C(3)	24(1)	38(1)	24(1)	5(1)	-1(1)	5(1)
C(4)	28(1)	49(1)	25(1)	17(1)	4(1)	12(1)
C(5)	28(1)	38(1)	27(1)	17(1)	8(1)	8(1)
C(6)	21(1)	32(1)	22(1)	9(1)	6(1)	8(1)
C(7)	20(1)	27(1)	20(1)	7(1)	8(1)	9(1)
C(8)	18(1)	23(1)	17(1)	9(1)	6(1)	8(1)
C(9)	22(1)	25(1)	17(1)	8(1)	6(1)	11(1)
C(10)	28(1)	33(1)	25(1)	12(1)	14(1)	17(1)
C(11)	22(1)	32(1)	36(1)	19(1)	14(1)	14(1)
C(12)	20(1)	23(1)	31(1)	8(1)	7(1)	6(1)
C(13)	21(1)	23(1)	18(1)	9(1)	5(1)	10(1)
C(14)	29(1)	30(1)	23(1)	1(1)	10(1)	12(1)
C(15)	30(1)	40(1)	58(2)	19(1)	26(1)	15(1)
C(16)	26(1)	24(1)	20(1)	4(1)	6(1)	8(1)
C(17)	19(1)	22(1)	16(1)	4(1)	5(1)	4(1)
C(18)	24(1)	35(1)	19(1)	7(1)	8(1)	11(1)
C(19)	27(1)	40(1)	21(1)	8(1)	13(1)	9(1)
C(20)	29(1)	25(1)	19(1)	4(1)	5(1)	0(1)
C(21)	24(1)	25(1)	22(1)	8(1)	2(1)	7(1)
C(22)	19(1)	23(1)	21(1)	5(1)	4(1)	4(1)
C(23)	40(1)	69(2)	32(1)	19(1)	22(1)	34(1)
C(24)	43(1)	40(1)	23(1)	12(1)	9(1)	7(1)
C(25)	34(1)	44(1)	34(1)	20(1)	17(1)	25(1)

Table 5. Hydrogen coordinates (Åx10^4) and isotropic displacement parameters (Å^{2}x10^3) for **1b**.

	x	y	z	U(eq)
H(2A)	9131	9777	5723	31
H(3A)	10386	9524	7628	39
H(4A)	9093	7709	8118	42
H(5A)	6550	6144	6709	38
H(6A)	5287	6386	4805	30
H(10A)	114	6958	4686	31
H(12A)	-1283	4078	1847	31
H(14A)	2455	8788	4988	42
H(14B)	3828	8878	4255	42
H(14C)	4065	8307	5394	42
H(15A)	-2332	4865	4402	59
H(15B)	-3127	3952	3072	59
H(15C)	-3393	5241	3278	59
H(16A)	513	3895	729	37
H(16B)	2623	4506	1452	37
H(16C)	1673	5173	566	37
H(19A)	6109	7643	-845	35
H(21A)	2281	8920	-475	31
H(23A)	7471	6776	512	61
H(23B)	6183	5972	1111	61
H(23C)	7643	7297	1885	61
H(24A)	3970	9504	-1938	55
H(24B)	2885	8093	-2670	55
H(24C)	5024	8651	-2283	55
H(25A)	1309	8944	1119	49
H(25B)	2721	9016	2370	49
H(25C)	1117	7744	1608	49

Table 6. Atomic coordinates (Å×10^4) and equivalent isotropic displacement parameters (Å^2×10^3) for **2b**. U(eq) is defined as one third of the trace of the orthogonalized U^{IJ} tensor.

	x	y	z	U(eq)
P(1)	5673(1)	1755(1)	8468(1)	21(1)
P(2)	3344(1)	1926(1)	7313(1)	21(1)
O(1)	4487(1)	3949(1)	7052(1)	21(1)
O(2)	3386(2)	6176(1)	7230(1)	24(1)
O(3)	2002(2)	4856(1)	7550(1)	23(1)
B(1)	3331(3)	4903(2)	7304(2)	21(1)
C(1)	7216(2)	2236(2)	8454(2)	23(1)
C(2)	8061(2)	1601(2)	9229(2)	32(1)
C(3)	9288(3)	1844(3)	9296(2)	41(1)
C(4)	9705(2)	2687(3)	8584(2)	36(1)
C(5)	8878(3)	3332(3)	7815(2)	38(1)
C(6)	7635(3)	3116(2)	7754(2)	32(1)
C(7)	4379(2)	2933(2)	9104(1)	22(1)
C(8)	3250(2)	2579(2)	9531(2)	28(1)
C(9)	2167(3)	3471(3)	9947(2)	34(1)
C(10)	2212(3)	4721(3)	9964(2)	35(1)
C(11)	3341(3)	5077(2)	9571(2)	31(1)
C(12)	4422(2)	4187(2)	9141(2)	25(1)
C(13)	2527(2)	2650(2)	6174(2)	22(1)
C(14)	1487(2)	2176(2)	6016(2)	31(1)
C(15)	752(3)	2677(3)	5195(2)	38(1)
C(16)	1018(3)	3665(3)	4519(2)	38(1)
C(17)	2015(3)	4163(3)	4670(2)	34(1)
C(18)	2764(2)	3668(2)	5487(2)	27(1)
C(19)	4191(2)	150(2)	7248(2)	24(1)
C(20)	4523(2)	-315(2)	6415(2)	28(1)
C(21)	5227(3)	-1666(2)	6429(2)	35(1)
C(22)	5621(3)	-2573(2)	7266(2)	38(1)
C(23)	5274(3)	-2132(2)	8095(2)	37(1)
C(24)	4551(2)	-782(2)	8084(2)	30(1)
C(25)	4932(2)	2501(2)	7247(2)	19(1)

C(26)	6040(2)	2026(2)	6517(2)	21(1)
C(27)	6893(2)	676(2)	6635(2)	26(1)
C(28)	7861(2)	217(2)	5949(2)	32(1)
C(29)	8006(2)	1086(3)	5142(2)	33(1)
C(30)	7207(2)	2438(3)	5031(2)	32(1)
C(31)	6237(2)	2907(2)	5711(2)	25(1)
C(32)	2047(2)	6944(2)	7482(2)	23(1)
C(33)	1564(3)	8262(2)	7567(2)	32(1)
C(34)	167(3)	8774(2)	7855(2)	37(1)
C(35)	-665(3)	7989(2)	8040(2)	37(1)
C(36)	-157(2)	6647(2)	7948(2)	30(1)
C(37)	1216(2)	6156(2)	7670(2)	23(1)

Table 7. Bond lengths [Å] and angles [°] for **2b**.

P(1)-C(7)	1.838(2)
P(1)-C(1)	1.842(2)
P(1)-C(25)	1.917(2)
P(2)-C(19)	1.838(2)
P(2)-C(13)	1.838(2)
P(2)-C(25)	1.940(2)
O(1)-B(1)	1.353(3)
O(1)-C(25)	1.445(2)
O(2)-B(1)	1.392(3)
O(2)-C(32)	1.395(3)
O(3)-B(1)	1.396(3)
O(3)-C(37)	1.399(2)
C(1)-C(6)	1.391(3)
C(1)-C(2)	1.400(3)
C(2)-C(3)	1.400(3)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.375(4)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.384(4)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.398(3)
C(5)-H(5A)	0.9500
C(6)-H(6A)	0.9500
C(7)-C(12)	1.401(3)
C(7)-C(8)	1.401(3)
C(8)-C(9)	1.387(3)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.389(4)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.388(4)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.395(3)
C(11)-H(11A)	0.9500
C(12)-H(12A)	0.9500

C(13)-C(18)	1.399(3)
C(13)-C(14)	1.407(3)
C(14)-C(15)	1.390(3)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.380(4)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.382(4)
C(16)-H(16A)	0.9500
C(17)-C(18)	1.393(3)
C(17)-H(17A)	0.9500
C(18)-H(18A)	0.9500
C(19)-C(24)	1.396(3)
C(19)-C(20)	1.405(3)
C(20)-C(21)	1.386(3)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.389(4)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.388(4)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.388(3)
C(23)-H(23A)	0.9500
C(24)-H(24A)	0.9500
C(25)-C(26)	1.522(3)
C(26)-C(27)	1.397(3)
C(26)-C(31)	1.399(3)
C(27)-C(28)	1.394(3)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.378(3)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.386(3)
C(29)-H(29A)	0.9500
C(30)-C(31)	1.391(3)
C(30)-H(30A)	0.9500
C(31)-H(31A)	0.9500
C(32)-C(33)	1.375(3)
C(32)-C(37)	1.388(3)

C(33)-C(34)	1.402(3)
C(33)-H(33A)	0.9500
C(34)-C(35)	1.386(4)
C(34)-H(34A)	0.9500
C(35)-C(36)	1.401(3)
C(35)-H(35A)	0.9500
C(36)-C(37)	1.374(3)
C(36)-H(36A)	0.9500
C(7)-P(1)-C(1)	102.05(10)
C(7)-P(1)-C(25)	99.37(9)
C(1)-P(1)-C(25)	105.42(10)
C(19)-P(2)-C(13)	101.41(10)
C(19)-P(2)-C(25)	101.87(9)
C(13)-P(2)-C(25)	105.89(10)
B(1)-O(1)-C(25)	132.31(17)
B(1)-O(2)-C(32)	104.52(17)
B(1)-O(3)-C(37)	104.01(16)
O(1)-B(1)-O(2)	117.6(2)
O(1)-B(1)-O(3)	129.6(2)
O(2)-B(1)-O(3)	112.51(18)
C(6)-C(1)-C(2)	117.8(2)
C(6)-C(1)-P(1)	127.16(18)
C(2)-C(1)-P(1)	115.00(18)
C(3)-C(2)-C(1)	121.0(2)
C(3)-C(2)-H(2A)	119.5
C(1)-C(2)-H(2A)	119.5
C(4)-C(3)-C(2)	120.2(2)
C(4)-C(3)-H(3A)	119.9
C(2)-C(3)-H(3A)	119.9
C(3)-C(4)-C(5)	119.6(2)
C(3)-C(4)-H(4A)	120.2
C(5)-C(4)-H(4A)	120.2
C(4)-C(5)-C(6)	120.4(2)
C(4)-C(5)-H(5A)	119.8
C(6)-C(5)-H(5A)	119.8
C(1)-C(6)-C(5)	120.9(2)

C(1)-C(6)-H(6A)	119.5
C(5)-C(6)-H(6A)	119.5
C(12)-C(7)-C(8)	118.6(2)
C(12)-C(7)-P(1)	123.67(17)
C(8)-C(7)-P(1)	117.65(17)
C(9)-C(8)-C(7)	120.8(2)
C(9)-C(8)-H(8A)	119.6
C(7)-C(8)-H(8A)	119.6
C(8)-C(9)-C(10)	119.8(2)
C(8)-C(9)-H(9A)	120.1
C(10)-C(9)-H(9A)	120.1
C(11)-C(10)-C(9)	120.3(2)
C(11)-C(10)-H(10A)	119.8
C(9)-C(10)-H(10A)	119.8
C(10)-C(11)-C(12)	119.8(2)
C(10)-C(11)-H(11A)	120.1
C(12)-C(11)-H(11A)	120.1
C(11)-C(12)-C(7)	120.5(2)
C(11)-C(12)-H(12A)	119.8
C(7)-C(12)-H(12A)	119.8
C(18)-C(13)-C(14)	117.5(2)
C(18)-C(13)-P(2)	127.04(17)
C(14)-C(13)-P(2)	115.27(18)
C(15)-C(14)-C(13)	121.1(2)
C(15)-C(14)-H(14A)	119.5
C(13)-C(14)-H(14A)	119.5
C(16)-C(15)-C(14)	120.5(2)
C(16)-C(15)-H(15A)	119.8
C(14)-C(15)-H(15A)	119.8
C(15)-C(16)-C(17)	119.3(2)
C(15)-C(16)-H(16A)	120.4
C(17)-C(16)-H(16A)	120.4
C(16)-C(17)-C(18)	120.9(2)
C(16)-C(17)-H(17A)	119.5
C(18)-C(17)-H(17A)	119.5
C(17)-C(18)-C(13)	120.7(2)

C(17)-C(18)-H(18A)	119.7
C(13)-C(18)-H(18A)	119.7
C(24)-C(19)-C(20)	118.6(2)
C(24)-C(19)-P(2)	117.21(17)
C(20)-C(19)-P(2)	124.20(18)
C(21)-C(20)-C(19)	120.3(2)
C(21)-C(20)-H(20A)	119.8
C(19)-C(20)-H(20A)	119.8
C(20)-C(21)-C(22)	120.3(2)
C(20)-C(21)-H(21A)	119.8
C(22)-C(21)-H(21A)	119.8
C(23)-C(22)-C(21)	120.0(2)
C(23)-C(22)-H(22A)	120.0
C(21)-C(22)-H(22A)	120.0
C(24)-C(23)-C(22)	119.8(2)
C(24)-C(23)-H(23A)	120.1
C(22)-C(23)-H(23A)	120.1
C(23)-C(24)-C(19)	120.9(2)
C(23)-C(24)-H(24A)	119.5
C(19)-C(24)-H(24A)	119.5
O(1)-C(25)-C(26)	106.78(17)
O(1)-C(25)-P(1)	110.78(13)
C(26)-C(25)-P(1)	110.69(14)
O(1)-C(25)-P(2)	110.60(13)
C(26)-C(25)-P(2)	115.19(14)
P(1)-C(25)-P(2)	102.83(10)
C(27)-C(26)-C(31)	117.9(2)
C(27)-C(26)-C(25)	120.3(2)
C(31)-C(26)-C(25)	121.82(19)
C(28)-C(27)-C(26)	120.7(2)
C(28)-C(27)-H(27A)	119.6
C(26)-C(27)-H(27A)	119.6
C(29)-C(28)-C(27)	120.8(2)
C(29)-C(28)-H(28A)	119.6
C(27)-C(28)-H(28A)	119.6
C(28)-C(29)-C(30)	119.1(2)

C(28)-C(29)-H(29A)	120.5
C(30)-C(29)-H(29A)	120.5
C(29)-C(30)-C(31)	120.6(2)
C(29)-C(30)-H(30A)	119.7
C(31)-C(30)-H(30A)	119.7
C(30)-C(31)-C(26)	120.8(2)
C(30)-C(31)-H(31A)	119.6
C(26)-C(31)-H(31A)	119.6
C(33)-C(32)-C(37)	122.7(2)
C(33)-C(32)-O(2)	128.0(2)
C(37)-C(32)-O(2)	109.31(18)
C(32)-C(33)-C(34)	115.8(2)
C(32)-C(33)-H(33A)	122.1
C(34)-C(33)-H(33A)	122.1
C(35)-C(34)-C(33)	121.5(2)
C(35)-C(34)-H(34A)	119.2
C(33)-C(34)-H(34A)	119.2
C(34)-C(35)-C(36)	121.9(2)
C(34)-C(35)-H(35A)	119.0
C(36)-C(35)-H(35A)	119.0
C(37)-C(36)-C(35)	116.0(2)
C(37)-C(36)-H(36A)	122.0
C(35)-C(36)-H(36A)	122.0
C(36)-C(37)-C(32)	122.1(2)
C(36)-C(37)-O(3)	128.3(2)
C(32)-C(37)-O(3)	109.59(18)

Symmetry transformations used to generate equivalent atoms:

Table 8. Anisotropic displacement parameters ($Å^2 x 10^3$) for **2b**. 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)	21(1)	22(1)	21(1)	-5(1)	-1(1)	-8(1)
P(2)	21(1)	22(1)	23(1)	-8(1)	2(1)	-9(1)
O(1)	21(1)	18(1)	23(1)	-6(1)	1(1)	-7(1)
O(2)	22(1)	19(1)	30(1)	-6(1)	0(1)	-6(1)
O(3)	23(1)	22(1)	26(1)	-7(1)	0(1)	-7(1)
B(1)	24(1)	21(1)	17(1)	-3(1)	-4(1)	-8(1)
C(1)	19(1)	26(1)	24(1)	-11(1)	0(1)	-5(1)
C(2)	28(1)	31(1)	36(1)	-2(1)	-7(1)	-9(1)
C(3)	31(1)	43(2)	47(2)	-6(1)	-16(1)	-8(1)
C(4)	20(1)	49(2)	47(2)	-24(1)	0(1)	-10(1)
C(5)	38(2)	55(2)	32(1)	-14(1)	5(1)	-29(1)
C(6)	33(1)	42(2)	25(1)	-6(1)	-2(1)	-21(1)
C(7)	24(1)	28(1)	15(1)	-7(1)	-2(1)	-9(1)
C(8)	31(1)	37(1)	20(1)	-6(1)	0(1)	-16(1)
C(9)	28(1)	53(2)	24(1)	-10(1)	4(1)	-15(1)
C(10)	28(1)	48(2)	25(1)	-16(1)	-2(1)	-2(1)
C(11)	34(1)	33(1)	27(1)	-14(1)	-7(1)	-4(1)
C(12)	24(1)	30(1)	21(1)	-6(1)	-5(1)	-8(1)
C(13)	20(1)	21(1)	25(1)	-12(1)	0(1)	-3(1)
C(14)	27(1)	27(1)	42(2)	-10(1)	-4(1)	-9(1)
C(15)	26(1)	36(2)	54(2)	-21(1)	-12(1)	-6(1)
C(16)	31(1)	44(2)	37(2)	-18(1)	-13(1)	-2(1)
C(17)	32(1)	38(2)	27(1)	-6(1)	-5(1)	-6(1)
C(18)	22(1)	32(1)	28(1)	-10(1)	-1(1)	-7(1)
C(19)	22(1)	21(1)	30(1)	-6(1)	0(1)	-11(1)
C(20)	29(1)	24(1)	31(1)	-9(1)	1(1)	-9(1)
C(21)	36(1)	27(1)	44(2)	-16(1)	1(1)	-10(1)
C(22)	32(1)	20(1)	63(2)	-9(1)	-10(1)	-7(1)
C(23)	42(2)	27(1)	45(2)	2(1)	-15(1)	-17(1)
C(24)	34(1)	29(1)	32(1)	-5(1)	-4(1)	-17(1)
C(25)	21(1)	16(1)	22(1)	-5(1)	1(1)	-6(1)

C(26)	17(1)	26(1)	22(1)	-9(1)	-1(1)	-9(1)
C(27)	22(1)	27(1)	29(1)	-9(1)	2(1)	-8(1)
C(28)	24(1)	32(1)	40(2)	-19(1)	2(1)	-6(1)
C(29)	24(1)	47(2)	29(1)	-19(1)	5(1)	-9(1)
C(30)	27(1)	48(2)	20(1)	-6(1)	3(1)	-13(1)
C(31)	20(1)	28(1)	25(1)	-4(1)	-2(1)	-6(1)
C(32)	23(1)	23(1)	21(1)	-5(1)	-2(1)	-5(1)
C(33)	38(1)	22(1)	34(1)	-7(1)	-2(1)	-7(1)
C(34)	41(2)	24(1)	36(2)	-8(1)	-1(1)	2(1)
C(35)	28(1)	35(2)	32(1)	-6(1)	2(1)	4(1)
C(36)	26(1)	33(1)	26(1)	-4(1)	1(1)	-6(1)
C(37)	25(1)	22(1)	18(1)	-4(1)	-4(1)	-4(1)

Table 9. Hydrogen coordinates (Åx10^4) and isotropic displacement parameters (Å^{2}x10^3) for **2b**.

	x	y	z	U(eq)
H(2A)	7797	997	9717	39
H(3A)	9835	1425	9835	49
H(4A)	10554	2827	8620	44
H(5A)	9156	3924	7326	45
H(6A)	7068	3577	7228	38
H(8A)	3227	1717	9535	34
H(9A)	1395	3229	10221	41
H(10A)	1466	5334	10245	42
H(11A)	3378	5925	9595	38
H(12A)	5193	4433	8871	30
H(14A)	1283	1503	6477	38
H(15A)	62	2336	5099	45
H(16A)	521	4000	3957	45
H(17A)	2193	4851	4210	41
H(18A)	3443	4026	5579	33
H(20A)	4263	300	5839	33
H(21A)	5441	-1974	5863	41
H(22A)	6127	-3494	7270	45
H(23A)	5531	-2753	8668	44
H(24A)	4297	-488	8654	36
H(27A)	6813	64	7190	31
H(28A)	8428	-706	6039	38
H(29A)	8645	763	4667	39
H(30A)	7324	3050	4486	39
H(31A)	5701	3838	5626	30
H(33A)	2142	8793	7438	38
H(34A)	-219	9679	7925	45
H(35A)	-1607	8372	8234	44
H(36A)	-728	6110	8070	36

Table 10. Atomic coordinates (Å×10^4) and equivalent isotropic displacement parameters (Å^2×10^3) for **2f**. U(eq) is defined as one third of the trace of the orthogonalized U^{IJ} tensor.

	x	y	z	U(eq)
P(1)	5844(1)	6300(1)	4229(1)	25(1)
P(2)	1613(1)	3299(1)	4327(1)	23(1)
P(3)	-489(1)	-20(1)	1034(1)	21(1)
P(4)	3493(1)	2059(1)	277(1)	23(1)
O(1)	2280(1)	4934(1)	3669(1)	22(1)
O(2)	1583(2)	5939(1)	3128(1)	34(1)
O(3)	1399(2)	6301(1)	4067(1)	27(1)
O(4)	3320(1)	1458(1)	1316(1)	21(1)
O(5)	4150(2)	-31(1)	1164(1)	28(1)
O(6)	4542(1)	1228(1)	1998(1)	26(1)
B(1)	1749(2)	5698(2)	3635(1)	24(1)
B(2)	3989(2)	890(2)	1475(1)	21(1)
C(1)	5529(2)	5530(2)	3508(1)	30(1)
C(2)	6138(3)	4799(2)	3351(1)	51(1)
C(3)	5975(4)	4157(3)	2823(2)	79(1)
C(4)	5198(4)	4232(3)	2440(2)	75(1)
C(5)	4581(3)	4940(3)	2579(1)	57(1)
C(6)	4740(2)	5598(2)	3113(1)	38(1)
C(7)	6727(2)	7774(2)	4160(1)	25(1)
C(8)	7622(2)	8406(2)	4574(1)	38(1)
C(9)	8286(2)	9547(2)	4573(1)	48(1)
C(10)	8072(2)	10071(2)	4166(1)	43(1)
C(11)	7207(3)	9457(2)	3749(1)	42(1)
C(12)	6541(2)	8313(2)	3745(1)	36(1)
C(13)	4397(2)	6462(2)	4404(1)	22(1)
C(14)	4588(2)	7382(2)	4918(1)	23(1)
C(15)	5178(2)	7392(3)	5404(1)	40(1)
C(16)	5340(3)	8252(3)	5864(1)	47(1)
C(17)	4901(3)	9103(2)	5846(1)	40(1)
C(18)	4294(3)	9086(2)	5370(1)	38(1)
C(19)	4150(2)	8237(2)	4910(1)	29(1)

C(20)	3520(2)	5333(2)	4491(1)	21(1)
C(21)	2554(2)	4666(2)	4168(1)	21(1)
C(22)	134(2)	3240(2)	4113(1)	22(1)
C(23)	-356(2)	2880(2)	3569(1)	30(1)
C(24)	-1497(2)	2803(2)	3443(1)	42(1)
C(25)	-2163(2)	3079(2)	3856(2)	49(1)
C(26)	-1688(3)	3455(2)	4395(2)	49(1)
C(27)	-545(2)	3534(2)	4524(1)	32(1)
C(28)	1852(2)	2308(2)	3747(1)	24(1)
C(29)	2738(2)	2616(2)	3384(1)	28(1)
C(30)	2877(2)	1809(2)	2960(1)	34(1)
C(31)	2117(3)	678(2)	2890(1)	39(1)
C(32)	1238(3)	362(2)	3248(1)	44(1)
C(33)	1115(2)	1158(2)	3676(1)	36(1)
C(34)	1298(3)	6970(2)	3241(1)	36(1)
C(35)	2462(3)	7972(2)	3266(1)	47(1)
C(36)	460(3)	6912(3)	2769(1)	59(1)
C(37)	758(2)	6900(2)	3816(1)	32(1)
C(38)	-548(3)	6154(3)	3774(2)	52(1)
C(39)	981(3)	8038(2)	4195(1)	44(1)
C(40)	-1312(2)	-965(2)	1496(1)	25(1)
C(41)	-2104(2)	-2054(2)	1245(1)	33(1)
C(42)	-2734(2)	-2837(2)	1561(1)	44(1)
C(43)	-2602(3)	-2558(3)	2129(1)	50(1)
C(44)	-1832(3)	-1487(3)	2385(1)	52(1)
C(45)	-1196(2)	-697(2)	2072(1)	38(1)
C(46)	-38(2)	1400(2)	1477(1)	22(1)
C(47)	871(2)	1863(2)	1901(1)	26(1)
C(48)	1086(2)	2933(2)	2225(1)	31(1)
C(49)	401(2)	3552(2)	2136(1)	35(1)
C(50)	-494(2)	3111(2)	1717(1)	37(1)
C(51)	-702(2)	2050(2)	1386(1)	29(1)
C(52)	921(2)	-339(2)	1013(1)	21(1)
C(53)	545(2)	-1615(2)	801(1)	24(1)
C(54)	553(2)	-2328(2)	1164(1)	35(1)
C(55)	104(3)	-3509(2)	989(2)	48(1)

C(56)	-366(3)	-3981(2)	452(2)	51(1)
C(57)	-372(2)	-3281(2)	84(1)	42(1)
C(58)	81(2)	-2105(2)	255(1)	30(1)
C(59)	1707(2)	376(2)	642(1)	20(1)
C(60)	2773(2)	1185(2)	781(1)	20(1)
C(61)	3290(2)	3408(2)	548(1)	25(1)
C(62)	3575(2)	4217(2)	206(1)	32(1)
C(63)	3407(2)	5236(2)	365(1)	40(1)
C(64)	2932(2)	5468(2)	858(1)	42(1)
C(65)	2640(3)	4674(2)	1202(1)	41(1)
C(66)	2825(2)	3655(2)	1049(1)	34(1)
C(67)	5074(2)	2432(2)	467(1)	24(1)
C(68)	5643(2)	1765(2)	172(1)	31(1)
C(69)	6855(2)	2060(2)	242(1)	37(1)
C(70)	7526(2)	3033(2)	606(1)	36(1)
C(71)	6984(2)	3698(2)	918(1)	35(1)
C(72)	5761(2)	3398(2)	847(1)	29(1)
C(73)	4706(2)	-479(2)	1548(1)	35(1)
C(74)	3668(3)	-1418(2)	1752(1)	49(1)
C(75)	5519(3)	-1004(3)	1258(1)	61(1)
C(76)	5294(2)	564(2)	2015(1)	30(1)
C(77)	6524(2)	1329(3)	1876(1)	48(1)
C(78)	5360(3)	331(3)	2590(1)	45(1)

Table 11. Bond lengths [Å] and angles [°] for **2f**.

P(1)-C(1)	1.835(3)
P(1)-C(7)	1.840(2)
P(1)-C(13)	1.883(2)
P(2)-C(21)	1.821(2)
P(2)-C(28)	1.831(2)
P(2)-C(22)	1.840(2)
P(3)-C(46)	1.834(2)
P(3)-C(40)	1.836(2)
P(3)-C(52)	1.895(2)
P(4)-C(60)	1.828(2)
P(4)-C(61)	1.837(3)
P(4)-C(67)	1.839(2)
O(1)-B(1)	1.363(3)
O(1)-C(21)	1.401(3)
O(2)-B(1)	1.367(3)
O(2)-C(34)	1.461(3)
O(3)-B(1)	1.359(3)
O(3)-C(37)	1.470(3)
O(4)-B(2)	1.363(3)
O(4)-C(60)	1.401(3)
O(5)-B(2)	1.362(3)
O(5)-C(73)	1.464(3)
O(6)-B(2)	1.372(3)
O(6)-C(76)	1.456(3)
C(1)-C(2)	1.393(4)
C(1)-C(6)	1.396(4)
C(2)-C(3)	1.381(5)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.369(6)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.370(6)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.399(4)
C(5)-H(5A)	0.9500

C(6)-H(6A)	0.9500
C(7)-C(12)	1.388(3)
C(7)-C(8)	1.393(3)
C(8)-C(9)	1.389(4)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.370(4)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.373(4)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.391(4)
C(11)-H(11A)	0.9500
C(12)-H(12A)	0.9500
C(13)-C(20)	1.505(3)
C(13)-C(14)	1.518(3)
C(13)-H(13A)	1.0000
C(14)-C(19)	1.379(3)
C(14)-C(15)	1.389(3)
C(15)-C(16)	1.388(4)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.379(4)
C(16)-H(16A)	0.9500
C(17)-C(18)	1.374(4)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.385(3)
C(18)-H(18A)	0.9500
C(19)-H(19A)	0.9500
C(20)-C(21)	1.328(3)
C(20)-H(20A)	0.9500
C(22)-C(23)	1.391(3)
C(22)-C(27)	1.392(3)
C(23)-C(24)	1.382(4)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.375(4)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.376(5)
C(25)-H(25A)	0.9500

C(26)-C(27)	1.385(4)
C(26)-H(26A)	0.9500
C(27)-H(27A)	0.9500
C(28)-C(29)	1.392(3)
C(28)-C(33)	1.397(3)
C(29)-C(30)	1.387(3)
C(29)-H(29A)	0.9500
C(30)-C(31)	1.386(4)
C(30)-H(30A)	0.9500
C(31)-C(32)	1.378(4)
C(31)-H(31A)	0.9500
C(32)-C(33)	1.377(4)
C(32)-H(32A)	0.9500
C(33)-H(33A)	0.9500
C(34)-C(36)	1.516(4)
C(34)-C(35)	1.519(4)
C(34)-C(37)	1.563(4)
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(39)	1.515(4)
C(37)-C(38)	1.519(4)
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-C(45)	1.391(4)
C(40)-C(41)	1.405(3)
C(41)-C(42)	1.384(4)
C(41)-H(41A)	0.9500
C(42)-C(43)	1.375(4)

C(42)-H(42A)	0.9500
C(43)-C(44)	1.384(4)
C(43)-H(43A)	0.9500
C(44)-C(45)	1.388(4)
C(44)-H(44A)	0.9500
C(45)-H(45A)	0.9500
C(46)-C(51)	1.391(3)
C(46)-C(47)	1.400(3)
C(47)-C(48)	1.389(3)
C(47)-H(47A)	0.9500
C(48)-C(49)	1.377(4)
C(48)-H(48A)	0.9500
C(49)-C(50)	1.382(4)
C(49)-H(49A)	0.9500
C(50)-C(51)	1.387(4)
C(50)-H(50A)	0.9500
C(51)-H(51A)	0.9500
C(52)-C(59)	1.499(3)
C(52)-C(53)	1.517(3)
C(52)-H(52A)	1.0000
C(53)-C(54)	1.385(3)
C(53)-C(58)	1.399(3)
C(54)-C(55)	1.392(4)
C(54)-H(54A)	0.9500
C(55)-C(56)	1.377(5)
C(55)-H(55A)	0.9500
C(56)-C(57)	1.383(4)
C(56)-H(56A)	0.9500
C(57)-C(58)	1.385(3)
C(57)-H(57A)	0.9500
C(58)-H(58A)	0.9500
C(59)-C(60)	1.330(3)
C(59)-H(59A)	0.9500
C(61)-C(66)	1.391(4)
C(61)-C(62)	1.395(3)
C(62)-C(63)	1.380(4)

C(62)-H(62A)	0.9500
C(63)-C(64)	1.376(4)
C(63)-H(63A)	0.9500
C(64)-C(65)	1.383(4)
C(64)-H(64A)	0.9500
C(65)-C(66)	1.388(4)
C(65)-H(65A)	0.9500
C(66)-H(66A)	0.9500
C(67)-C(68)	1.391(3)
C(67)-C(72)	1.392(3)
C(68)-C(69)	1.381(4)
C(68)-H(68A)	0.9500
C(69)-C(70)	1.374(4)
C(69)-H(69A)	0.9500
C(70)-C(71)	1.384(4)
C(70)-H(70A)	0.9500
C(71)-C(72)	1.394(3)
C(71)-H(71A)	0.9500
C(72)-H(72A)	0.9500
C(73)-C(75)	1.497(4)
C(73)-C(76)	1.541(4)
C(73)-C(74)	1.551(4)
C(74)-H(74A)	0.9800
C(74)-H(74B)	0.9800
C(74)-H(74C)	0.9800
C(75)-H(75A)	0.9800
C(75)-H(75B)	0.9800
C(75)-H(75C)	0.9800
C(76)-C(78)	1.502(4)
C(76)-C(77)	1.539(4)
C(77)-H(77A)	0.9800
C(77)-H(77B)	0.9800
C(77)-H(77C)	0.9800
C(78)-H(78A)	0.9800
C(78)-H(78B)	0.9800
C(78)-H(78C)	0.9800

C(1)-P(1)-C(7)	102.97(11)
C(1)-P(1)-C(13)	102.71(11)
C(7)-P(1)-C(13)	99.82(10)
C(21)-P(2)-C(28)	100.87(10)
C(21)-P(2)-C(22)	101.33(10)
C(28)-P(2)-C(22)	100.69(10)
C(46)-P(3)-C(40)	102.69(11)
C(46)-P(3)-C(52)	103.44(10)
C(40)-P(3)-C(52)	100.12(10)
C(60)-P(4)-C(61)	101.78(11)
C(60)-P(4)-C(67)	102.47(10)
C(61)-P(4)-C(67)	101.75(11)
B(1)-O(1)-C(21)	123.72(19)
B(1)-O(2)-C(34)	105.57(19)
B(1)-O(3)-C(37)	105.71(19)
B(2)-O(4)-C(60)	121.94(18)
B(2)-O(5)-C(73)	105.46(18)
B(2)-O(6)-C(76)	105.96(18)
O(3)-B(1)-O(1)	126.3(2)
O(3)-B(1)-O(2)	115.0(2)
O(1)-B(1)-O(2)	118.6(2)
O(5)-B(2)-O(4)	126.1(2)
O(5)-B(2)-O(6)	114.6(2)
O(4)-B(2)-O(6)	119.2(2)
C(2)-C(1)-C(6)	118.0(3)
C(2)-C(1)-P(1)	115.4(2)
C(6)-C(1)-P(1)	126.6(2)
C(3)-C(2)-C(1)	121.5(4)
C(3)-C(2)-H(2A)	119.3
C(1)-C(2)-H(2A)	119.3
C(4)-C(3)-C(2)	119.9(4)
C(4)-C(3)-H(3A)	120.0
C(2)-C(3)-H(3A)	120.0
C(3)-C(4)-C(5)	120.3(3)
C(3)-C(4)-H(4A)	119.9

C(5)-C(4)-H(4A)	119.9
C(4)-C(5)-C(6)	120.4(4)
C(4)-C(5)-H(5A)	119.8
C(6)-C(5)-H(5A)	119.8
C(1)-C(6)-C(5)	120.0(3)
C(1)-C(6)-H(6A)	120.0
C(5)-C(6)-H(6A)	120.0
C(12)-C(7)-C(8)	117.9(2)
C(12)-C(7)-P(1)	125.42(19)
C(8)-C(7)-P(1)	116.62(19)
C(9)-C(8)-C(7)	120.6(3)
C(9)-C(8)-H(8A)	119.7
C(7)-C(8)-H(8A)	119.7
C(10)-C(9)-C(8)	120.7(3)
C(10)-C(9)-H(9A)	119.7
C(8)-C(9)-H(9A)	119.7
C(9)-C(10)-C(11)	119.7(3)
C(9)-C(10)-H(10A)	120.2
C(11)-C(10)-H(10A)	120.2
C(10)-C(11)-C(12)	120.1(3)
C(10)-C(11)-H(11A)	120.0
C(12)-C(11)-H(11A)	120.0
C(7)-C(12)-C(11)	121.1(3)
C(7)-C(12)-H(12A)	119.5
C(11)-C(12)-H(12A)	119.5
C(20)-C(13)-C(14)	111.10(18)
C(20)-C(13)-P(1)	109.21(15)
C(14)-C(13)-P(1)	110.01(15)
C(20)-C(13)-H(13A)	108.8
C(14)-C(13)-H(13A)	108.8
P(1)-C(13)-H(13A)	108.8
C(19)-C(14)-C(15)	117.9(2)
C(19)-C(14)-C(13)	119.5(2)
C(15)-C(14)-C(13)	122.5(2)
C(16)-C(15)-C(14)	120.7(3)
C(16)-C(15)-H(15A)	119.7

C(14)-C(15)-H(15A)	119.7
C(17)-C(16)-C(15)	120.4(3)
C(17)-C(16)-H(16A)	119.8
C(15)-C(16)-H(16A)	119.8
C(18)-C(17)-C(16)	119.3(3)
C(18)-C(17)-H(17A)	120.4
C(16)-C(17)-H(17A)	120.4
C(17)-C(18)-C(19)	120.1(3)
C(17)-C(18)-H(18A)	119.9
C(19)-C(18)-H(18A)	119.9
C(14)-C(19)-C(18)	121.5(2)
C(14)-C(19)-H(19A)	119.2
C(18)-C(19)-H(19A)	119.2
C(21)-C(20)-C(13)	127.0(2)
C(21)-C(20)-H(20A)	116.5
C(13)-C(20)-H(20A)	116.5
C(20)-C(21)-O(1)	121.5(2)
C(20)-C(21)-P(2)	120.90(18)
O(1)-C(21)-P(2)	117.39(15)
C(23)-C(22)-C(27)	118.4(2)
C(23)-C(22)-P(2)	123.83(18)
C(27)-C(22)-P(2)	117.69(19)
C(24)-C(23)-C(22)	120.6(2)
C(24)-C(23)-H(23A)	119.7
C(22)-C(23)-H(23A)	119.7
C(25)-C(24)-C(23)	120.3(3)
C(25)-C(24)-H(24A)	119.9
C(23)-C(24)-H(24A)	119.9
C(24)-C(25)-C(26)	120.0(3)
C(24)-C(25)-H(25A)	120.0
C(26)-C(25)-H(25A)	120.0
C(25)-C(26)-C(27)	120.0(3)
C(25)-C(26)-H(26A)	120.0
C(27)-C(26)-H(26A)	120.0
C(26)-C(27)-C(22)	120.7(3)
C(26)-C(27)-H(27A)	119.7

C(22)-C(27)-H(27A)	119.7
C(29)-C(28)-C(33)	117.9(2)
C(29)-C(28)-P(2)	124.42(18)
C(33)-C(28)-P(2)	117.60(19)
C(30)-C(29)-C(28)	121.0(2)
C(30)-C(29)-H(29A)	119.5
C(28)-C(29)-H(29A)	119.5
C(31)-C(30)-C(29)	120.0(3)
C(31)-C(30)-H(30A)	120.0
C(29)-C(30)-H(30A)	120.0
C(32)-C(31)-C(30)	119.5(3)
C(32)-C(31)-H(31A)	120.3
C(30)-C(31)-H(31A)	120.3
C(33)-C(32)-C(31)	120.6(3)
C(33)-C(32)-H(32A)	119.7
C(31)-C(32)-H(32A)	119.7
C(32)-C(33)-C(28)	120.9(3)
C(32)-C(33)-H(33A)	119.5
C(28)-C(33)-H(33A)	119.5
O(2)-C(34)-C(36)	107.8(2)
O(2)-C(34)-C(35)	106.4(2)
C(36)-C(34)-C(35)	111.1(2)
O(2)-C(34)-C(37)	102.08(19)
C(36)-C(34)-C(37)	115.4(3)
C(35)-C(34)-C(37)	113.1(2)
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5

H(36B)-C(36)-H(36C)	109.5
O(3)-C(37)-C(39)	108.2(2)
O(3)-C(37)-C(38)	106.7(2)
C(39)-C(37)-C(38)	110.4(2)
O(3)-C(37)-C(34)	101.9(2)
C(39)-C(37)-C(34)	115.4(2)
C(38)-C(37)-C(34)	113.4(2)
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(45)-C(40)-C(41)	117.7(2)
C(45)-C(40)-P(3)	125.31(19)
C(41)-C(40)-P(3)	116.96(19)
C(42)-C(41)-C(40)	121.0(3)
C(42)-C(41)-H(41A)	119.5
C(40)-C(41)-H(41A)	119.5
C(43)-C(42)-C(41)	120.5(3)
C(43)-C(42)-H(42A)	119.8
C(41)-C(42)-H(42A)	119.8
C(42)-C(43)-C(44)	119.5(3)
C(42)-C(43)-H(43A)	120.2
C(44)-C(43)-H(43A)	120.2
C(43)-C(44)-C(45)	120.4(3)
C(43)-C(44)-H(44A)	119.8
C(45)-C(44)-H(44A)	119.8
C(44)-C(45)-C(40)	120.9(3)
C(44)-C(45)-H(45A)	119.5

C(40)-C(45)-H(45A)	119.5
C(51)-C(46)-C(47)	118.0(2)
C(51)-C(46)-P(3)	115.60(17)
C(47)-C(46)-P(3)	126.41(19)
C(48)-C(47)-C(46)	120.7(2)
C(48)-C(47)-H(47A)	119.7
C(46)-C(47)-H(47A)	119.7
C(49)-C(48)-C(47)	120.5(2)
C(49)-C(48)-H(48A)	119.8
C(47)-C(48)-H(48A)	119.8
C(48)-C(49)-C(50)	119.6(2)
C(48)-C(49)-H(49A)	120.2
C(50)-C(49)-H(49A)	120.2
C(49)-C(50)-C(51)	120.2(3)
C(49)-C(50)-H(50A)	119.9
C(51)-C(50)-H(50A)	119.9
C(50)-C(51)-C(46)	121.1(2)
C(50)-C(51)-H(51A)	119.5
C(46)-C(51)-H(51A)	119.5
C(59)-C(52)-C(53)	113.84(19)
C(59)-C(52)-P(3)	106.99(15)
C(53)-C(52)-P(3)	106.09(14)
C(59)-C(52)-H(52A)	109.9
C(53)-C(52)-H(52A)	109.9
P(3)-C(52)-H(52A)	109.9
C(54)-C(53)-C(58)	118.7(2)
C(54)-C(53)-C(52)	119.9(2)
C(58)-C(53)-C(52)	121.1(2)
C(53)-C(54)-C(55)	120.7(3)
C(53)-C(54)-H(54A)	119.7
C(55)-C(54)-H(54A)	119.7
C(56)-C(55)-C(54)	120.0(3)
C(56)-C(55)-H(55A)	120.0
C(54)-C(55)-H(55A)	120.0
C(55)-C(56)-C(57)	120.1(3)
C(55)-C(56)-H(56A)	120.0

C(57)-C(56)-H(56A)	120.0
C(56)-C(57)-C(58)	120.1(3)
C(56)-C(57)-H(57A)	120.0
C(58)-C(57)-H(57A)	120.0
C(57)-C(58)-C(53)	120.5(3)
C(57)-C(58)-H(58A)	119.8
C(53)-C(58)-H(58A)	119.8
C(60)-C(59)-C(52)	127.0(2)
C(60)-C(59)-H(59A)	116.5
C(52)-C(59)-H(59A)	116.5
C(59)-C(60)-O(4)	122.23(19)
C(59)-C(60)-P(4)	118.99(17)
O(4)-C(60)-P(4)	118.54(15)
C(66)-C(61)-C(62)	118.2(2)
C(66)-C(61)-P(4)	125.16(19)
C(62)-C(61)-P(4)	116.59(19)
C(63)-C(62)-C(61)	120.7(3)
C(63)-C(62)-H(62A)	119.6
C(61)-C(62)-H(62A)	119.6
C(64)-C(63)-C(62)	120.7(2)
C(64)-C(63)-H(63A)	119.6
C(62)-C(63)-H(63A)	119.6
C(63)-C(64)-C(65)	119.4(3)
C(63)-C(64)-H(64A)	120.3
C(65)-C(64)-H(64A)	120.3
C(64)-C(65)-C(66)	120.2(3)
C(64)-C(65)-H(65A)	119.9
C(66)-C(65)-H(65A)	119.9
C(65)-C(66)-C(61)	120.8(2)
C(65)-C(66)-H(66A)	119.6
C(61)-C(66)-H(66A)	119.6
C(68)-C(67)-C(72)	117.9(2)
C(68)-C(67)-P(4)	117.56(18)
C(72)-C(67)-P(4)	124.23(19)
C(69)-C(68)-C(67)	121.5(2)
C(69)-C(68)-H(68A)	119.3

C(67)-C(68)-H(68A)	119.3
C(70)-C(69)-C(68)	120.0(3)
C(70)-C(69)-H(69A)	120.0
C(68)-C(69)-H(69A)	120.0
C(69)-C(70)-C(71)	120.0(2)
C(69)-C(70)-H(70A)	120.0
C(71)-C(70)-H(70A)	120.0
C(70)-C(71)-C(72)	119.8(2)
C(70)-C(71)-H(71A)	120.1
C(72)-C(71)-H(71A)	120.1
C(67)-C(72)-C(71)	120.8(2)
C(67)-C(72)-H(72A)	119.6
C(71)-C(72)-H(72A)	119.6
O(5)-C(73)-C(75)	110.8(2)
O(5)-C(73)-C(76)	103.16(19)
C(75)-C(73)-C(76)	116.0(2)
O(5)-C(73)-C(74)	105.2(2)
C(75)-C(73)-C(74)	109.3(2)
C(76)-C(73)-C(74)	111.6(2)
C(73)-C(74)-H(74A)	109.5
C(73)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5
C(73)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5
H(74B)-C(74)-H(74C)	109.5
C(73)-C(75)-H(75A)	109.5
C(73)-C(75)-H(75B)	109.5
H(75A)-C(75)-H(75B)	109.5
C(73)-C(75)-H(75C)	109.5
H(75A)-C(75)-H(75C)	109.5
H(75B)-C(75)-H(75C)	109.5
O(6)-C(76)-C(78)	109.2(2)
O(6)-C(76)-C(77)	105.4(2)
C(78)-C(76)-C(77)	110.0(2)
O(6)-C(76)-C(73)	102.72(18)
C(78)-C(76)-C(73)	116.8(2)

C(77)-C(76)-C(73)	111.9(2)
C(76)-C(77)-H(77A)	109.5
C(76)-C(77)-H(77B)	109.5
H(77A)-C(77)-H(77B)	109.5
C(76)-C(77)-H(77C)	109.5
H(77A)-C(77)-H(77C)	109.5
H(77B)-C(77)-H(77C)	109.5
C(76)-C(78)-H(78A)	109.5
C(76)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
C(76)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 12. Anisotropic displacement parameters ($Å^2 x 10^3$) for **2f**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	23(1)	20(1)	28(1)	3(1)	2(1)	6(1)
P(2)	24(1)	20(1)	25(1)	8(1)	2(1)	6(1)
P(3)	19(1)	21(1)	22(1)	3(1)	0(1)	6(1)
P(4)	21(1)	25(1)	22(1)	7(1)	2(1)	6(1)
O(1)	25(1)	19(1)	19(1)	5(1)	0(1)	7(1)
O(2)	59(1)	24(1)	22(1)	3(1)	-5(1)	21(1)
O(3)	36(1)	26(1)	24(1)	6(1)	1(1)	17(1)
O(4)	20(1)	22(1)	21(1)	3(1)	0(1)	6(1)
O(5)	36(1)	31(1)	19(1)	-1(1)	-4(1)	19(1)
O(6)	30(1)	30(1)	19(1)	0(1)	-2(1)	14(1)
B(1)	25(1)	20(1)	23(1)	4(1)	-4(1)	3(1)
B(2)	18(1)	19(1)	21(1)	1(1)	2(1)	4(1)
C(1)	30(1)	22(1)	30(1)	1(1)	10(1)	1(1)
C(2)	62(2)	39(2)	54(2)	2(2)	18(2)	23(2)
C(3)	117(4)	56(2)	66(3)	-4(2)	33(3)	41(2)
C(4)	111(4)	44(2)	43(2)	-10(2)	33(2)	6(2)
C(5)	59(2)	57(2)	28(2)	5(2)	6(1)	-10(2)
C(6)	34(2)	39(2)	30(2)	3(1)	7(1)	1(1)
C(7)	22(1)	23(1)	28(1)	2(1)	3(1)	8(1)
C(8)	31(1)	31(1)	48(2)	6(1)	-9(1)	7(1)
C(9)	30(2)	31(2)	71(2)	-2(2)	-10(1)	3(1)
C(10)	33(2)	23(1)	69(2)	10(1)	17(1)	6(1)
C(11)	51(2)	33(2)	44(2)	16(1)	14(1)	14(1)
C(12)	40(2)	33(2)	32(2)	8(1)	1(1)	8(1)
C(13)	23(1)	20(1)	21(1)	3(1)	-1(1)	6(1)
C(14)	20(1)	23(1)	22(1)	3(1)	2(1)	4(1)
C(15)	47(2)	50(2)	29(2)	-3(1)	-8(1)	31(1)
C(16)	48(2)	60(2)	30(2)	-10(1)	-12(1)	26(2)
C(17)	44(2)	34(2)	32(2)	-8(1)	6(1)	10(1)
C(18)	51(2)	29(1)	35(2)	6(1)	12(1)	17(1)
C(19)	36(1)	26(1)	24(1)	5(1)	2(1)	12(1)

C(20)	23(1)	19(1)	22(1)	5(1)	3(1)	10(1)
C(21)	23(1)	20(1)	22(1)	5(1)	4(1)	10(1)
C(22)	24(1)	15(1)	26(1)	6(1)	7(1)	5(1)
C(23)	30(1)	29(1)	32(1)	4(1)	3(1)	11(1)
C(24)	31(1)	37(2)	55(2)	8(1)	-11(1)	9(1)
C(25)	21(1)	37(2)	93(3)	24(2)	7(2)	10(1)
C(26)	40(2)	37(2)	80(3)	21(2)	34(2)	21(1)
C(27)	39(2)	24(1)	33(2)	6(1)	16(1)	10(1)
C(28)	23(1)	22(1)	30(1)	8(1)	1(1)	12(1)
C(29)	29(1)	23(1)	33(1)	6(1)	1(1)	11(1)
C(30)	42(2)	38(2)	32(2)	6(1)	5(1)	25(1)
C(31)	50(2)	34(2)	39(2)	-5(1)	-9(1)	28(1)
C(32)	44(2)	21(1)	65(2)	4(1)	-5(2)	13(1)
C(33)	32(1)	23(1)	54(2)	11(1)	9(1)	11(1)
C(34)	57(2)	23(1)	30(1)	3(1)	-9(1)	20(1)
C(35)	65(2)	29(2)	51(2)	17(1)	10(2)	18(2)
C(36)	95(3)	47(2)	43(2)	1(2)	-28(2)	38(2)
C(37)	37(1)	26(1)	40(2)	8(1)	-3(1)	16(1)
C(38)	39(2)	41(2)	81(3)	18(2)	-4(2)	17(1)
C(39)	61(2)	35(2)	43(2)	2(1)	2(1)	29(2)
C(40)	18(1)	26(1)	33(1)	7(1)	4(1)	9(1)
C(41)	23(1)	30(1)	42(2)	7(1)	4(1)	7(1)
C(42)	32(2)	31(2)	65(2)	13(2)	12(1)	6(1)
C(43)	42(2)	44(2)	65(2)	28(2)	25(2)	12(1)
C(44)	58(2)	54(2)	40(2)	18(2)	20(2)	11(2)
C(45)	38(2)	36(2)	34(2)	7(1)	9(1)	5(1)
C(46)	21(1)	23(1)	21(1)	5(1)	3(1)	6(1)
C(47)	28(1)	25(1)	23(1)	3(1)	-1(1)	9(1)
C(48)	32(1)	32(1)	22(1)	2(1)	0(1)	6(1)
C(49)	43(2)	27(1)	30(2)	-3(1)	4(1)	11(1)
C(50)	41(2)	31(1)	42(2)	0(1)	-2(1)	19(1)
C(51)	28(1)	29(1)	32(1)	4(1)	-2(1)	13(1)
C(52)	17(1)	22(1)	22(1)	4(1)	1(1)	6(1)
C(53)	18(1)	18(1)	37(1)	5(1)	7(1)	6(1)
C(54)	31(1)	29(1)	49(2)	13(1)	10(1)	11(1)
C(55)	47(2)	31(2)	74(2)	25(2)	23(2)	17(1)

C(56)	42(2)	23(1)	85(3)	4(2)	28(2)	10(1)
C(57)	29(1)	30(2)	54(2)	-8(1)	12(1)	4(1)
C(58)	22(1)	26(1)	37(2)	1(1)	7(1)	7(1)
C(59)	20(1)	20(1)	21(1)	4(1)	1(1)	8(1)
C(60)	20(1)	20(1)	21(1)	4(1)	2(1)	9(1)
C(61)	18(1)	25(1)	31(1)	10(1)	1(1)	5(1)
C(62)	28(1)	32(1)	36(2)	16(1)	5(1)	5(1)
C(63)	40(2)	26(1)	54(2)	22(1)	5(1)	7(1)
C(64)	40(2)	23(1)	61(2)	8(1)	2(1)	11(1)
C(65)	46(2)	30(2)	48(2)	7(1)	14(1)	16(1)
C(66)	39(2)	28(1)	37(2)	14(1)	13(1)	13(1)
C(67)	22(1)	25(1)	24(1)	10(1)	5(1)	6(1)
C(68)	33(1)	29(1)	32(1)	6(1)	4(1)	14(1)
C(69)	37(2)	42(2)	43(2)	14(1)	11(1)	24(1)
C(70)	23(1)	46(2)	46(2)	25(1)	8(1)	13(1)
C(71)	25(1)	35(2)	40(2)	7(1)	-2(1)	5(1)
C(72)	26(1)	31(1)	28(1)	5(1)	2(1)	10(1)
C(73)	46(2)	39(2)	28(1)	2(1)	-7(1)	28(1)
C(74)	56(2)	35(2)	58(2)	10(2)	-3(2)	18(2)
C(75)	83(2)	85(3)	39(2)	-3(2)	-1(2)	68(2)
C(76)	28(1)	41(2)	23(1)	4(1)	0(1)	18(1)
C(77)	31(2)	60(2)	50(2)	13(2)	0(1)	13(1)
C(78)	51(2)	61(2)	32(2)	11(2)	-4(1)	27(2)

Table 13. Hydrogen coordinates (Åx10^4) and isotropic displacement parameters (Å^{2}x10^3) for **2f**.

	x	y	z	U(eq)
H(2A)	6678	4740	3614	62
H(3A)	6400	3664	2725	95
H(4A)	5087	3791	2076	90
H(5A)	4042	4986	2311	68
H(6A)	4312	6090	3206	46
H(8A)	7781	8054	4858	46
H(9A)	8893	9968	4858	58
H(10A)	8521	10855	4172	51
H(11A)	7062	9815	3464	51
H(12A)	5949	7894	3453	44
H(13A)	4085	6695	4088	26
H(15A)	5474	6803	5424	48
H(16A)	5756	8255	6192	56
H(17A)	5016	9693	6159	48
H(18A)	3973	9659	5356	45
H(19A)	3740	8243	4581	35
H(20A)	3673	5069	4810	25
H(23A)	98	2686	3282	36
H(24A)	-1822	2558	3070	51
H(25A)	-2953	3010	3768	58
H(26A)	-2143	3662	4678	59
H(27A)	-223	3791	4897	38
H(29A)	3257	3392	3427	33
H(30A)	3493	2032	2718	41
H(31A)	2201	124	2597	47
H(32A)	713	-411	3200	52
H(33A)	520	922	3927	43
H(35A)	2847	7878	2921	70
H(35B)	2982	7999	3579	70
H(35C)	2310	8684	3315	70
H(36A)	871	6946	2426	88

H(36B)	193	7558	2852	88
H(36C)	-227	6194	2723	88
H(38A)	-796	6029	4143	79
H(38B)	-676	5417	3532	79
H(38C)	-1013	6533	3619	79
H(39A)	654	7908	4552	66
H(39B)	597	8470	4025	66
H(39C)	1835	8474	4253	66
H(41A)	-2210	-2256	852	39
H(42A)	-3260	-3572	1383	52
H(43A)	-3037	-3097	2345	60
H(44A)	-1738	-1291	2778	63
H(45A)	-674	37	2253	46
H(47A)	1347	1442	1967	31
H(48A)	1710	3240	2509	37
H(49A)	543	4278	2363	42
H(50A)	-968	3535	1654	45
H(51A)	-1308	1763	1094	35
H(52A)	1321	-132	1394	25
H(54A)	868	-2008	1535	42
H(55A)	121	-3991	1240	58
H(56A)	-685	-4787	335	61
H(57A)	-688	-3608	-287	50
H(58A)	76	-1628	0	36
H(59A)	1412	235	267	24
H(62A)	3887	4063	-140	39
H(63A)	3623	5785	131	48
H(64A)	2805	6166	962	50
H(65A)	2311	4827	1543	49
H(66A)	2631	3120	1290	40
H(68A)	5188	1091	-82	37
H(69A)	7224	1590	37	44
H(70A)	8362	3249	645	43
H(71A)	7444	4356	1180	42
H(72A)	5392	3857	1060	34
H(74A)	3171	-1952	1432	74

H(74B)	3193	-1063	1983	74
H(74C)	3986	-1831	1970	74
H(75A)	6091	-448	1071	91
H(75B)	5055	-1681	984	91
H(75C)	5942	-1227	1529	91
H(77A)	6772	2074	2126	72
H(77B)	6486	1432	1492	72
H(77C)	7097	967	1923	72
H(78A)	4559	-72	2693	68
H(78B)	5726	1055	2851	68
H(78C)	5837	-143	2599	68

Table 14. Atomic coordinates ($Å \times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **3a**. U(eq) is defined as one third of the trace of the orthogonalized U^{IJ} tensor.

	x	y	z	U(eq)
Rh(1)	5230.5(2)	5546.9(2)	6846.5(2)	19.64(5)
P(2)	3204.6(6)	5263.9(4)	7216.5(6)	16.19(12)
P(1)	4348.9(6)	5266.6(4)	5097.9(6)	18.60(13)
O(1)	1651.0(14)	5504.3(15)	5214.1(13)	19.7(3)
O(3)	1669.7(19)	5175.0(11)	3099.6(16)	25.1(4)
O(2)	11.9(19)	5907.1(12)	3841.7(17)	26.3(4)
C(32)	2828(3)	4424.6(16)	8159(2)	18.9(5)
C(2)	2257(2)	4137.7(15)	5497(2)	18.4(5)
C(3)	3147(3)	3536.1(15)	5736(2)	21.7(5)
C(14)	4973(3)	4501.3(16)	4123(2)	25.6(6)
C(26)	2116(3)	6018.0(14)	7781(2)	19.2(5)
C(21)	3693(3)	6802.2(16)	4518(3)	28.3(6)
C(1)	2645(2)	4988.5(14)	5611(2)	16.7(5)
C(22)	3607(3)	7461.2(17)	3784(3)	34.9(7)
C(33)	3864(3)	4008.1(16)	8663(2)	24.3(5)
C(4)	2771(3)	2759.0(16)	5653(3)	29.1(6)
C(23)	4025(3)	7430.3(19)	2620(3)	36.2(8)
C(37)	1577(3)	4165.0(17)	8359(2)	25.1(6)
C(20)	4161(3)	6102.0(15)	4074(2)	21.4(5)
C(7)	982(3)	3933.0(17)	5220(2)	24.8(6)
C(30)	79(3)	6679(2)	8016(3)	44.5(9)
B(1)	1148(2)	5523(3)	4071(2)	20.0(5)
C(31)	797(3)	6079(2)	7518(3)	34.6(7)
C(19)	6252(3)	4283(2)	4298(3)	38.7(8)
C(13)	438(4)	6739(2)	2173(3)	39.7(9)
C(9)	1438(4)	5379(2)	968(3)	46.1(10)
C(28)	1948(3)	7127.8(18)	9106(3)	36.1(7)
C(8)	708(3)	5245.8(18)	2117(3)	31.7(6)
C(25)	4577(3)	6076.0(18)	2899(3)	33.6(7)
C(29)	664(4)	7209.0(19)	8792(3)	39.1(8)
C(35)	2404(3)	3088.4(18)	9529(3)	33.9(7)
C(34)	3645(3)	3343.2(18)	9353(3)	31.5(6)

C(36)	1371(3)	3501.6(19)	9037(3)	31.9(7)
C(5)	1520(3)	2563.5(18)	5343(3)	34.6(7)
C(12)	-1549(4)	5909(3)	2186(4)	51.2(10)
C(27)	2676(3)	6542.1(17)	8588(3)	28.1(7)
C(24)	4518(4)	6739(2)	2182(3)	41.8(8)
C(6)	621(3)	3151.6(19)	5135(3)	34.0(7)
C(17)	6012(5)	3335(2)	2713(4)	59.7(12)
C(15)	4216(4)	4136.3(18)	3230(3)	36.2(7)
C(10)	-18(4)	4474(2)	2065(4)	47.7(10)
C(11)	-125(3)	5954.3(18)	2535(3)	30.0(6)
C(18)	6780(4)	3704(2)	3584(4)	57.1(12)
C(16)	4748(5)	3552(2)	2538(3)	53.5(11)
C(47)	6801(2)	5509(3)	8475(3)	35.1(6)
C(42)	7421(3)	5253.9(19)	7414(3)	34.6(7)
C(48)	6306(3)	6281(2)	8255(3)	33.4(7)
C(41)	7275(3)	5876(2)	6545(3)	34.9(7)
C(40)	6682(3)	6521.6(18)	7099(3)	34.7(7)
C(46)	6771(4)	5007(3)	9486(4)	53.4(11)
C(43)	7996(3)	4504(2)	7388(4)	53.3(11)
C(45)	7350(5)	4304(3)	9439(5)	68.8(15)
C44)	7952(4)	4045(2)	8422(6)	70.9(16)

Table 15. Bond lengths [Å] and angles [°] for **3a**.

Rh(1)-P(2)	2.1991(7)
Rh(1)-P(1)	2.1847(7)
Rh(1)-C(47)	2.406(3)
Rh(1)-C(42)	2.388(3)
Rh(1)-C(48)	2.277(3)
Rh(1)-C(41)	2.221(3)
Rh(1)-C(40)	2.253(3)
P(2)-C(32)	1.825(3)
P(2)-C(26)	1.832(3)
P(2)-C(1)	1.927(2)
P(1)-C(14)	1.828(3)
P(1)-C(1)	1.926(3)
P(1)-C(20)	1.834(3)
O(1)-C(1)	1.415(3)
O(1)-B(1)	1.365(3)
O(3)-B(1)	1.360(3)
O(3)-C(8)	1.466(3)
O(2)-B(1)	1.363(4)
O(2)-C(11)	1.464(3)
C(32)-C(33)	1.391(4)
C(32)-C(37)	1.390(4)
C(2)-C(3)	1.400(4)
C(2)-C(1)	1.511(3)
C(2)-C(7)	1.390(4)
C(3)-C(4)	1.384(4)
C(14)-C(19)	1.383(4)
C(14)-C(15)	1.397(4)
C(26)-C(31)	1.391(4)
C(26)-C(27)	1.385(4)
C(21)-C(22)	1.392(4)
C(21)-C(20)	1.385(4)
C(22)-C(23)	1.381(5)

C(33)-C(34)	1.392(4)
C(4)-C(5)	1.371(5)
C(23)-C(24)	1.380(5)
C(37)-C(36)	1.381(4)
C(20)-C(25)	1.391(4)
C(7)-C(6)	1.387(4)
C(30)-C(31)	1.388(4)
C(30)-C(29)	1.381(5)
C(19)-C(18)	1.390(5)
C(13)-C(11)	1.519(5)
C(9)-C(8)	1.522(4)
C(28)-C(29)	1.371(5)
C(28)-C(27)	1.387(4)
C(8)-C(10)	1.516(5)
C(8)-C(11)	1.563(4)
C(25)-C(24)	1.387(4)
C(35)-C(34)	1.374(4)
C(35)-C(36)	1.382(5)
C(5)-C(6)	1.384(5)
C(12)-C(11)	1.515(5)
C(17)-C(18)	1.389(7)
C(17)-C(16)	1.368(7)
C(15)-C(16)	1.384(5)
C(47)-C(42)	1.429(5)
C(47)-C(48)	1.433(6)
C(47)-C(46)	1.417(5)
C(42)-C(41)	1.443(5)
C(42)-C(43)	1.412(5)
C(48)-C(40)	1.417(5)
C(41)-C(40)	1.412(5)
C(46)-C(45)	1.343(7)
C(43)-C(44)	1.397(7)
C(45)-C(44)	1.380(8)
P(2)-Rh(1)-C(47)	118.66(7)
P(2)-Rh(1)-C(42)	143.64(8)
P(2)-Rh(1)-C(48)	116.21(8)

P(2)-Rh(1)-C(41)	177.20(9)
P(2)-Rh(1)-C(40)	140.65(9)
P(1)-Rh(1)-P(2)	75.08(2)
P(1)-Rh(1)-C(47)	157.84(10)
P(1)-Rh(1)-C(42)	124.15(9)
P(1)-Rh(1)-C(48)	157.15(9)
P(1)-Rh(1)-C(41)	107.23(9)
P(1)-Rh(1)-C(40)	122.29(9)
C(42)-Rh(1)-C(47)	34.67(11)
C(48)-Rh(1)-C(47)	35.50(14)
C(48)-Rh(1)-C(42)	59.31(11)
C(41)-Rh(1)-C(47)	59.67(11)
C(41)-Rh(1)-C(42)	36.25(11)
C(41)-Rh(1)-C(48)	61.06(12)
C(41)-Rh(1)-C(40)	36.78(12)
C(40)-Rh(1)-C(47)	59.41(13)
C(40)-Rh(1)-C(42)	59.83(11)
C(40)-Rh(1)-C(48)	36.45(12)
C(32)-P(2)-Rh(1)	119.95(9)
C(32)-P(2)-C(26)	102.15(12)
C(32)-P(2)-C(1)	106.34(11)
C(26)-P(2)-Rh(1)	120.47(9)
C(26)-P(2)-C(1)	108.60(11)
C(1)-P(2)-Rh(1)	98.24(8)
C(14)-P(1)-Rh(1)	122.85(10)
C(14)-P(1)-C(1)	109.90(12)
C(14)-P(1)-C(20)	102.59(12)
C(1)-P(1)-Rh(1)	98.75(8)
C(20)-P(1)-Rh(1)	114.90(9)
C(20)-P(1)-C(1)	107.07(11)
B(1)-O(1)-C(1)	124.2(2)
B(1)-O(3)-C(8)	106.6(2)
B(1)-O(2)-C(11)	105.9(2)
C(33)-C(32)-P(2)	117.4(2)
C(37)-C(32)-P(2)	123.8(2)
C(37)-C(32)-C(33)	118.8(3)

C(3)-C(2)-C(1)	121.1(2)
C(7)-C(2)-C(3)	118.2(2)
C(7)-C(2)-C(1)	120.5(2)
C(4)-C(3)-C(2)	120.5(3)
C(19)-C(14)-P(1)	117.3(2)
C(19)-C(14)-C(15)	119.8(3)
C(15)-C(14)-P(1)	122.9(2)
C(31)-C(26)-P(2)	126.0(2)
C(27)-C(26)-P(2)	115.3(2)
C(27)-C(26)-C(31)	118.7(3)
C(20)-C(21)-C(22)	120.3(3)
P(1)-C(1)-P(2)	87.78(11)
O(1)-C(1)-P(2)	109.69(16)
O(1)-C(1)-P(1)	114.59(17)
O(1)-C(1)-C(2)	112.5(2)
C(2)-C(1)-P(2)	112.63(16)
C(2)-C(1)-P(1)	117.06(17)
C(23)-C(22)-C(21)	120.4(3)
C(32)-C(33)-C(34)	120.3(3)
C(5)-C(4)-C(3)	120.7(3)
C(24)-C(23)-C(22)	119.6(3)
C(36)-C(37)-C(32)	120.5(3)
C(21)-C(20)-P(1)	118.7(2)
C(21)-C(20)-C(25)	118.9(3)
C(25)-C(20)-P(1)	122.1(2)
C(6)-C(7)-C(2)	120.6(3)
C(29)-C(30)-C(31)	120.3(3)
O(3)-B(1)-O(1)	125.8(3)
O(3)-B(1)-O(2)	114.7(2)
O(2)-B(1)-O(1)	119.5(2)
C(30)-C(31)-C(26)	120.1(3)
C(14)-C(19)-C(18)	119.9(4)
C(29)-C(28)-C(27)	119.9(3)
O(3)-C(8)-C(9)	107.5(3)
O(3)-C(8)-C(10)	106.4(3)
O(3)-C(8)-C(11)	102.1(2)

C(9)-C(8)-C(11)	115.1(3)
C(10)-C(8)-C(9)	110.7(3)
C(10)-C(8)-C(11)	114.0(3)
C(24)-C(25)-C(20)	120.5(3)
C(28)-C(29)-C(30)	120.0(3)
C(34)-C(35)-C(36)	119.8(3)
C(35)-C(34)-C(33)	120.2(3)
C(37)-C(36)-C(35)	120.5(3)
C(4)-C(5)-C(6)	119.4(3)
C(26)-C(27)-C(28)	120.9(3)
C(23)-C(24)-C(25)	120.2(3)
C(5)-C(6)-C(7)	120.5(3)
C(16)-C(17)-C(18)	120.2(3)
C(16)-C(15)-C(14)	119.7(4)
O(2)-C(11)-C(13)	106.6(2)
O(2)-C(11)-C(8)	102.4(2)
O(2)-C(11)-C(12)	108.7(3)
C(13)-C(11)-C(8)	112.7(3)
C(12)-C(11)-C(13)	110.7(3)
C(12)-C(11)-C(8)	115.0(3)
C(17)-C(18)-C(19)	119.9(4)
C(17)-C(16)-C(15)	120.5(4)
C(42)-C(47)-Rh(1)	71.99(15)
C(42)-C(47)-C(48)	107.7(3)
C(48)-C(47)-Rh(1)	67.33(16)
C(46)-C(47)-Rh(1)	126.1(2)
C(46)-C(47)-C(42)	119.7(4)
C(46)-C(47)-C(48)	132.6(4)
C(47)-C(42)-Rh(1)	73.34(15)
C(47)-C(42)-C(41)	107.0(3)
C(41)-C(42)-Rh(1)	65.56(16)
C(43)-C(42)-Rh(1)	125.5(2)
C(43)-C(42)-C(47)	119.5(4)
C(43)-C(42)-C(41)	133.5(4)
C(47)-C(48)-Rh(1)	77.18(17)
C(40)-C(48)-Rh(1)	70.86(17)

C(40)-C(48)-C(47)	108.5(3)
C(42)-C(41)-Rh(1)	78.19(17)
C(40)-C(41)-Rh(1)	72.83(17)
C(40)-C(41)-C(42)	108.6(3)
C(48)-C(40)-Rh(1)	72.69(17)
C(41)-C(40)-Rh(1)	70.39(17)
C(41)-C(40)-C(48)	107.8(3)
C(45)-C(46)-C(47)	119.3(5)
C(44)-C(43)-C(42)	117.9(4)
C(46)-C(45)-C(44)	122.0(4)
C(45)-C(44)-C(43)	121.6(4)

Table 16. Anisotropic displacement parameters ($Å^2x10^3$) for **3a**. 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}
Rh(1)	16.77(8)	19.77(8)	22.37(9)	0.34(10)	0.25(6)	-0.18(10)
P(2)	16.7(3)	17.4(3)	14.5(3)	-1.6(2)	-0.1(2)	1.1(2)
P(1)	20.9(3)	16.5(3)	18.6(3)	0.5(2)	4.3(2)	2.2(2)
O(1)	22.9(7)	18.4(8)	17.5(7)	-1.3(9)	-2.5(6)	5.9(10)
O(3)	32.7(10)	25.2(9)	17.3(9)	-1.8(7)	-3.2(7)	3.9(8)
O(2)	28.2(10)	30.6(10)	19.9(9)	1.0(8)	-5.6(8)	6.8(8)
C(32)	22.4(13)	19.7(13)	14.6(12)	-2.3(10)	0.8(10)	-1.0(10)
C(2)	23.6(13)	18.9(12)	12.8(11)	-1.4(9)	2.3(9)	-0.5(10)
C(3)	25.7(13)	20.1(12)	19.5(12)	-0.9(10)	2.2(10)	1.8(10)
C(14)	36.3(16)	18.6(13)	22.5(13)	1.7(10)	11.7(11)	4.7(11)
C(26)	22.5(12)	18.7(12)	16.7(12)	-0.6(9)	4.2(9)	3.1(10)
C(21)	34.1(16)	21.4(13)	29.5(15)	0.5(11)	2.4(12)	-0.8(12)
C(1)	20.2(12)	17.3(11)	12.6(11)	-0.7(9)	0.9(9)	3.2(10)
C(22)	38.5(18)	18.7(14)	47.6(19)	3.6(13)	1.0(14)	2.8(13)
C(33)	24.6(14)	25.6(14)	22.8(13)	1.1(11)	0.0(10)	1.8(11)
C(4)	38.0(17)	18.9(13)	30.6(15)	0.5(11)	5.9(13)	2.5(12)
C(23)	37.8(18)	28.8(16)	42.0(19)	16.3(14)	1.5(15)	-3.3(14)
C(37)	23.7(14)	32.0(15)	19.6(13)	-0.1(11)	-0.2(10)	-0.1(11)
C(20)	23.2(13)	18.7(12)	22.3(13)	4.2(10)	1.4(10)	-1.7(10)
C(7)	23.7(13)	24.6(13)	26.1(14)	1.5(11)	-0.4(11)	-0.3(11)
C(30)	34.9(18)	61(2)	37.5(18)	-9.3(16)	0.9(14)	23.9(17)
B(1)	23.8(12)	17.0(11)	19.2(11)	0.1(15)	-1.8(9)	0.0(17)
C(31)	27.6(15)	46.3(19)	29.7(15)	-14.8(14)	-3.1(12)	10.9(14)
C(19)	36.9(17)	35.2(17)	44.8(19)	5.8(14)	15.8(14)	11.3(14)
C(13)	57(2)	33.0(18)	29.3(16)	5.7(14)	-3.5(16)	5.0(17)
C(9)	72(2)	47(3)	18.6(13)	-1.6(13)	1.2(14)	11.1(18)
C(28)	44.5(19)	24.4(15)	40.5(18)	-12.8(13)	18.5(15)	-9.4(14)
C(8)	45.5(17)	29.2(14)	19.8(13)	-2.2(11)	-11.5(12)	-0.9(14)
C(25)	44.5(18)	27.0(14)	29.9(16)	4.2(12)	9.7(13)	2.4(13)
C(29)	51(2)	29.1(16)	37.8(18)	-2.7(14)	18.6(15)	15.4(15)
C(35)	44.1(19)	28.4(15)	29.4(15)	7.7(12)	6.6(13)	-0.8(13)
C(34)	35.0(16)	31.2(15)	28.2(15)	6.7(12)	-0.5(12)	7.0(13)
C(36)	30.7(16)	37.7(17)	27.5(15)	3.6(12)	4.2(12)	-8.7(13)

C(5)	45.3(19)	20.5(14)	38.1(17)	-2.0(12)	5.4(14)	-9.1(13)
C(12)	41(2)	65(2)	46(2)	0.7(18)	-20.4(16)	4.7(18)
C(27)	28.3(15)	24.1(15)	32.1(16)	-8.7(12)	6.0(12)	-6.3(12)
C(24)	53(2)	38.8(18)	33.9(18)	14.9(15)	12.5(15)	-0.6(16)
C(6)	30.3(16)	32.3(16)	39.3(17)	1.7(13)	-2.4(13)	-10.8(13)
C(17)	88(3)	40(2)	53(2)	-6.8(18)	36(2)	20(2)
C(15)	50(2)	31.6(16)	27.8(15)	-6.0(13)	8.2(14)	6.3(14)
C(10)	63(3)	35(2)	43(2)	-4.7(16)	-21.0(18)	-8.7(19)
C(11)	35.8(16)	33.1(16)	20.4(14)	1.2(11)	-10.1(12)	4.2(13)
C(18)	57(2)	48(2)	68(3)	9(2)	34(2)	28(2)
C(16)	90(3)	36.0(19)	36(2)	-10.8(15)	22(2)	5(2)
C(47)	25.1(12)	39.7(15)	39.8(14)	0.5(19)	-11.8(10)	-13.0(18)
C(42)	16.4(12)	31.6(14)	55(2)	-1.4(14)	-8.8(13)	-4.2(11)
C(48)	21.8(14)	37.8(17)	40.2(17)	-9.5(14)	-4.8(12)	-5.9(13)
C(41)	21.6(14)	40.0(16)	43.4(19)	0.2(14)	4.6(13)	-8.6(13)
C(40)	27.3(16)	26.5(15)	50(2)	2.7(14)	-5.8(14)	-6.5(12)
C(46)	50(2)	63(3)	45(2)	11.3(18)	-27.9(17)	-25(2)
C(43)	21.3(16)	41(2)	97(3)	-11(2)	-16.2(18)	2.9(14)
C(45)	64(3)	52(3)	87(4)	27(3)	-53(3)	-22(2)
C(44)	42(2)	32(2)	136(5)	15(3)	-52(3)	-1.9(17)

Table 17. Hydrogen coordinates (Åx10^4) and isotropic displacement parameters (Å^{2}x10^3) for **3a**.

	x	y	z	U(eq)
H(3)	4016.4	3662.12	5956.54	26
H(21)	3428.71	6832.78	5325.31	34
H(22)	3258.86	7934.72	4086.62	42
H(33)	4724.16	4178.1	8536.71	29
H(4)	3386.94	2356.56	5812.73	35
H(23)	3974.19	7882.35	2124.44	43
H(37)	860.1	4445.91	8027.48	30
H(7)	352.97	4331.7	5087.79	30
H(30)	-818.03	6724.37	7822.09	53
H(31)	386.39	5710.17	6996.75	42
H(19)	6769.99	4528.36	4905.87	46
H(13A)	-9.29	7161.55	2589.78	60
H(13B)	323.35	6809.61	1304.73	60
H(13C)	1362.04	6753.48	2390.25	60
H(9A)	2030.96	5822.96	1076.87	69
H(9B)	819.96	5492.97	309.65	69
H(9C)	1932.42	4907.51	776.84	69
H(28)	2338.04	7472.26	9678.55	43
H(25)	4903.66	5599.94	2586.17	40
H(29)	177.31	7629.8	9107.98	47
H(35)	2256.36	2629.8	9988.56	41
H(34)	4355.6	3064.85	9701.53	38
H(36)	512.15	3328.09	9164.6	38
H(5)	1273.42	2029	5271.98	41
H1(2A)	-1920.42	5429.99	2519.87	77
H(12B)	-1649.36	5899.36	1310.51	77
H(12C)	-1998.62	6366.55	2502.73	77
H(27)	3572.17	6499.79	8788.9	34
H(24)	4818.62	6717.45	1385.18	50
H(6)	-250.55	3019.32	4932.8	41
H(17)	6366.87	2929.88	2238.7	72
H(15)	3339.52	4288.44	3098.86	43
H(10A)	601.41	4040.51	2038.58	72

H(10B)	-581.53	4461.7	1345.2	72
H(10C)	-544.63	4422.05	2778.58	72
H(18)	7663.22	3561.18	3690.2	69
H(16)	4231.14	3299.96	1935.79	64
H(48)	5809.71	6581.6	8792.25	40
H(41)	7534.93	5853.86	5735.05	42
H(40)	6557.59	7027.01	6758.28	42
H(46)	6346.26	5167.14	10190.22	64
H(43)	8401.31	4317.71	6688.36	64
H(45)	7346.18	3974.74	10125.29	83
H(44)	8344.83	3541.59	8426.32	85

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