

**SUPPORTING INFORMATION of SYNTHESSES, STRUCTURES,
AND COMPUTATIONS**

**Protonation of carbene-stabilized diphosphorus:
complexation of HP_2^+**

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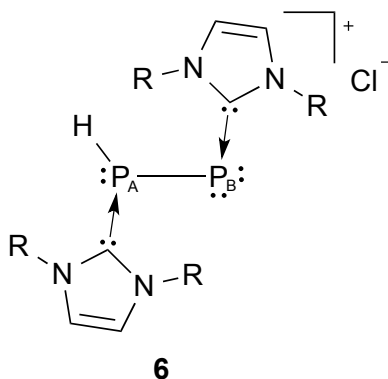
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SUPPORTING INFORMATIONs of SYNTHESSES

Materials and Methods

General.

The syntheses of air-sensitive compounds were performed under purified argon using Schlenk techniques and an inert atmosphere drybox (M-Braun LabMaster SP). Pyridine hydrochloride (from Aldrich) was washed with anhydrous diethyl ether and dried in vacuo. All the other chemicals were purchased from Aldrich and Strem and used as received. The solvents were dried and distilled under argon from Na/benzophenone prior to use. ^1H NMR, $^{13}\text{C}\{^1\text{H}\}$ NMR, ^{31}P and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra were recorded on a Varian Unity Inova 500 MHz spectrometer. The chemical shifts were referenced to an external H_3PO_4 standard for ^{31}P NMR spectra. Electrochemistry measurements were performed with a PAR Model 273A potentiostat using a non-aqueous Ag/Ag^+ (0.01 M $\text{AgNO}_3/0.1$ M $n\text{-Bu}_4\text{NPF}_6$ in MeCN) reference electrode, Pt-wire counter electrode, and a Glassy Carbon working milli-electrode (diameter = 2 mm) under an argon atmosphere. Measurements were performed at ambient temperature using 5.0 mM analyte in THF containing 0.1 M $n\text{-Bu}_4\text{NPF}_6$ as the supporting electrolyte. Ferrocene (Fc) was used as an external standard and all potentials are reported relative to the Fc^+/Fc couple. X-ray intensity data for $\mathbf{6} \cdot (\text{THF})_2$ were collected on a Bruker SMART APEX II X-ray diffractometer system with graphite-monochromated Mo K radiation ($\lambda = 0.71073 \text{ \AA}$), using the ω -scan technique.



Compound **6**: 20 mL of toluene was added to a Schlenk flask containing both **5** (0.29 g, 0.35 mmol) and $\text{HCl} \cdot \text{NC}_5\text{H}_5$ (0.04 g, 0.35 mmol), which was then stirred overnight at room temperature. After filtration, the residue was rinsed with 30 mL of toluene and then dried in vacuo, giving compound **6** as yellow powder (0.30 g, 99.3% yield). Mp: decomposed ($> 218^\circ\text{C}$) and melt (at 272°C). X-ray quality colorless crystals of **6** were obtained by recrystallization of **6** in the THF/hexane mixed solvent. ^1H NMR (499.8 MHz, THF-d_8): δ 0.87 [d, 6H, $\text{CH}(\text{CH}_3)_2$], 0.93 [d, 6H, $\text{CH}(\text{CH}_3)_2$], 1.01 [d, 6H, $\text{CH}(\text{CH}_3)_2$], 1.07 [m, 24H, $\text{CH}(\text{CH}_3)_2$], 1.17 [d, 6H, $\text{CH}(\text{CH}_3)_2$], 2.07 [m, 2H, $\text{CH}(\text{CH}_3)_2$], 2.18 [m, 2H, $\text{CH}(\text{CH}_3)_2$], 2.51 [m, 2H, $\text{CH}(\text{CH}_3)_2$], 2.63 [m, 2H, $\text{CH}(\text{CH}_3)_2$], 3.51 (dd, $|^1J_{\text{P(A)}-\text{H}}| = 205 \text{ Hz}$, $|^2J_{\text{P(B)}-\text{H}}| = 10 \text{ Hz}$, 1H, PH) 7.11 (d, 2H, Ar-H), 7.15 (d, 2H, Ar-H), 7.22

(d, 2H, Ar-*H*), 7.24 (d, 2H, Ar-*H*), 7.35 (t, 2H, Ar-*H*), 7.37 (s, 2H, NCH), 7.42 (t, 2H, Ar-*H*), 9.24 (s, 2H, NCH). $^{13}\text{C}\{^1\text{H}\}$ NMR (125.7 MHz, THF- d_8): δ 23.1 [CH(CH₃)₂], 23.2 [CH(CH₃)₂], 23.6 [br, CH(CH₃)₂], 23.8 [CH(CH₃)₂], 25.0 [CH(CH₃)₂], 26.20 and 26.24 [CH(CH₃)₂], 29.7 [CH(CH₃)₂], 29.83 and 29.85 [CH(CH₃)₂], 30.1 [br, CH(CH₃)₂], 124.2, 131.2 (NCH), 124.9, 125.1, 125.2, 125.3, 131.7, 131.9, 133.1, 134.30, 134.32, 145.9, 146.7, 147.3, 149.5 (Ar-*C*), 152.6 [dd, $|^1J_{\text{P(A)-C}}| = 48.5$ Hz, $|^2J_{\text{P(B)-C}}| = 27.0$ Hz, NCP_A(H)P_B], 170.1 [dd, $|^1J_{\text{P(B)-C}}| = 117.9$ Hz, $|^2J_{\text{P(A)-C}}| = 14.5$ Hz, NCP_BP_A(H)]. ^{31}P NMR (THF- d_8 , 202.3 MHz): δ -105.2 (P_A), -109.8 (P_B) ($|^1J_{\text{PP}}| = 235$ Hz, $|^1J_{\text{P(A)-H}}| = 204$ Hz, $|^2J_{\text{P(B)-H}}| = 11$ Hz). Crystal data for **6**·(THF)₂: C₆₂H₈₉N₄O₂P₂Cl, fw = 1019.76, monoclinic, $P2_1/n$, $a = 12.974(3)$ Å, $b = 31.717(7)$ Å, $c = 15.286(3)$ Å, $\beta = 95.960(3)^\circ$, $V = 6256(2)$ Å³, $Z = 4$, $R1 = 0.0775$ for 6441 data ($I > 2\sigma(I)$), $wR_2 = 0.2193$ (all data).

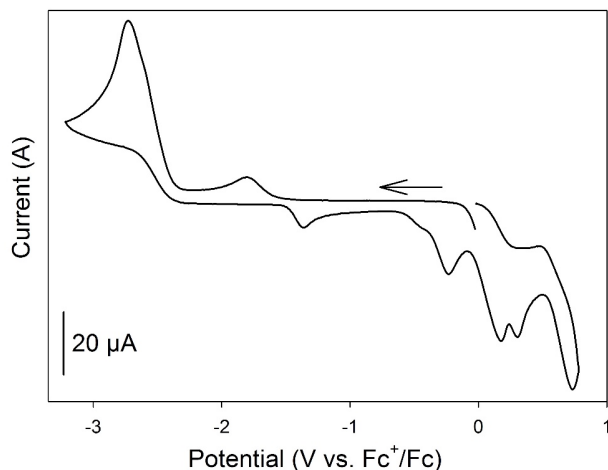


Figure S1. Diffusion-controlled cyclic voltammogram of a 5 mM THF solution of compound **6**. Conditions: scan speed: 100 mV/s; 0.1 $n\text{Bu}_4\text{NPF}_6$ supporting electrolyte, glassy carbon working electrode, Pt-wire counter electrode, RT. Arrow displays direction of scan [Note: The peak at -2.73 V may correspond to the irreversible reduction of the LH^+Cl^- [$\text{L}: = \text{:C}\{\text{N}(2,6\text{-Pr}_i_2\text{C}_6\text{H}_3)\text{CH}\}_2$] salt.¹ This salt was formed in situ due to the moisture that was introduced into the cell during the measurement. The peak at -0.24 V may correspond to the oxidation of the carbene ligand [$\text{L}: = \text{:C}\{\text{N}(2,6\text{-Pr}_i_2\text{C}_6\text{H}_3)\text{CH}\}_2$], which was produced in situ from the irreversible reduction of the corresponding imidazolium chloride salt].¹

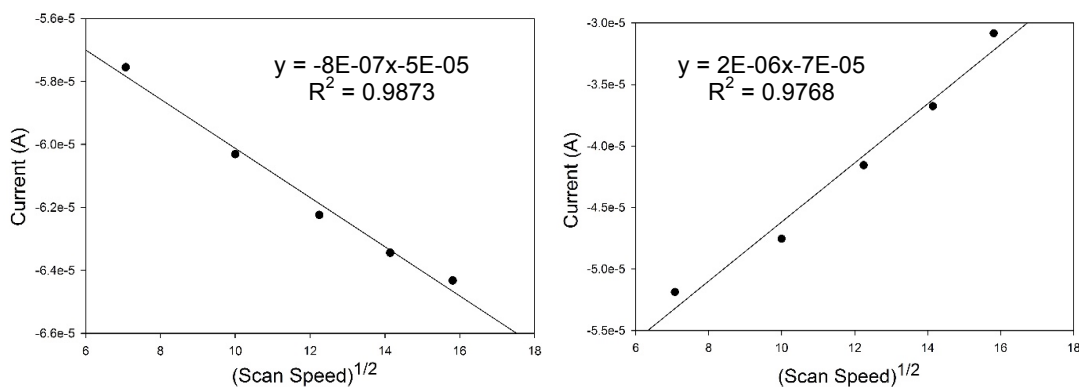


Figure S2. Plots of the square root of scan speed vs. current (A) for the anodic (*left*) and cathodic (*right*) currents for the quasi-reversible redox couple for compound **6** at $E_{1/2} = -1.60$ V (vs. Fc^+/Fc) at 100 mV/s.

Reference:

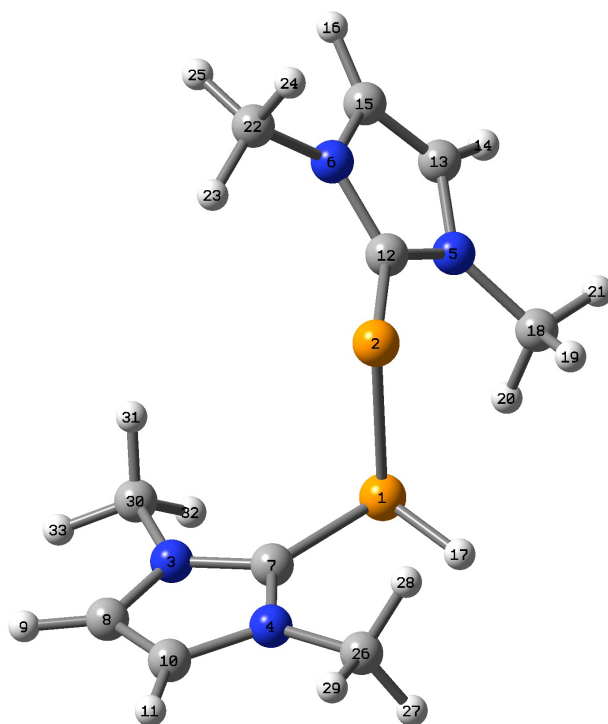
- 1 T. M. Ramnial, The Chemistry of Imidazolium Salts and Phosphonium-Based Ionic Liquids. Ph.D. Thesis, Simon Fraser University, 2006.

SUPPORTING INFORMATIONS of COMPUTATIONS

All computations employed the Gaussian 94 and Gaussian09 programs:

For Gaussian 94: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Gill, P. M. W.; Johnson, B. G.; Robb, M. A.; Cheeseman, J. R.; Keith, T.; Petersson, G. A.; Montgomery, J. A.; Raghavachari, K.; Al-Laham, M. A.; Zakrzewski, V. G.; Ortiz, J. V.; Foresman, J. B.; Peng, C. Y.; Ayala, P. Y.; Chen, W.; Wong, M. W.; Andes, J. L.; Replogle, E. S.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Binkley, J. S.; Defrees, D. J.; Baker, J.; Stewart, J. J. P.; Head-Gordon, M.; Gonzalez, C.; Pople, J. A. Gaussian 94, Revision B.3; Gaussian Inc.: Pittsburgh, PA, 1995.

For Gaussian 09: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09*, revision D.01; Gaussian, Inc., Wallingford CT, 2013.



[6-Me]⁺

Fig. S3 The simplified model **[6-Me]⁺** [L: = :C{N(Me)CH}₂]. Selected bond distances (Å) and angles (deg): P(1)–C(7) = 1.841, P(1)–P(2) = 2.225, P(2)–C(12) = 1.815; C(7)–P(1)–P(2) = 99.3, P(1)–P(2)–C(12) = 99.0, C(7)–P(1)–H(17) = 93.5, H(17)–P(1)–P(2) = 102.8.

Table S1. Coordinates of the B3LYP/6-311+G** optimized geometry of [6-Me]⁺

P	-0.65252706	-1.15683516	-0.50371385
P	0.53411103	-0.33243674	1.18891253
N	-2.39806226	1.03022663	-0.90198312
N	-3.30428794	-0.42614547	0.42784113
N	2.84815276	-0.85423591	-0.50646720
N	2.90071148	1.02554780	0.58444364
C	-2.18927810	-0.16468925	-0.29881416
C	-3.63661236	1.52356238	-0.54649145
H	-4.00339244	2.46845134	-0.90849238
C	-4.20777205	0.60904228	0.27730087
H	-5.16871823	0.60509653	0.76201085
C	2.10759646	-0.05958143	0.32575345
C	4.07084101	-0.25854529	-0.76791962
H	4.80028550	-0.71235158	-1.41624595
C	4.11011454	0.90312928	-0.07456975
H	4.88407137	1.64686335	0.00402876
H	-1.22882986	-2.32585069	0.05669584
C	2.49696940	-2.20110935	-0.94942475
H	1.97348604	-2.71221047	-0.13994846
H	1.86530923	-2.17650556	-1.83741596
H	3.41655341	-2.73984568	-1.17442303
C	2.55283121	2.13902671	1.46372205
H	1.47486144	2.29408700	1.42237553
H	2.83779641	1.92162621	2.49486028
H	3.07505700	3.03233319	1.12279754
C	-3.54675651	-1.61266251	1.25763015
H	-3.73994848	-2.48496298	0.63300207
H	-2.68791279	-1.79789326	1.90061774
H	-4.41840147	-1.41702302	1.87885678
C	-1.43129946	1.72537076	-1.75418268
H	-0.65181258	2.17787539	-1.13937677
H	-0.98128922	1.01464934	-2.44665787
H	-1.95627793	2.49572651	-2.31553113

SUPPORTING INFORMATIONs of X-RAY

Compound 6·(THF)₂

A specimen of C₆₂H₈₉ClN₄O₂P₂, approximate dimensions 0.120 mm x 0.200 mm x 0.420 mm in an orange crystal sealed in a glass capillary under an argon atmosphere in the drybox, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at room temperature on a Bruker SMART APEX II CCD X-ray diffractometer system with graphite-monochromated Mo K α radiation (λ = 0.71073 Å, sealed tube) using ω -scan technique.

The total exposure time was 7.00 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 67749 reflections to a maximum θ angle of 25.25° (0.83 Å resolution), of which 11336 were independent (average redundancy 5.976, completeness = 99.9%, R_{int} = 9.65%, R_{sig} = 6.38%) and 6441 (56.82%) were greater than $2\sigma(F^2)$. The final cell constants of a = 12.974(3) Å, b = 31.717(7) Å, c = 15.286(3) Å, β = 95.960(3)°, volume = 6256(2) Å³, are based upon the refinement of the XYZ-centroids of 6780 reflections above $20\sigma(I)$ with $4.34^\circ < 2\theta < 40.66^\circ$. The data were corrected for Lorentz and polarization effects and integrated with the manufacturer's SAINT software. Absorption corrections were applied with the multi-scan method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6127 and 0.7454.

The structure was solved and refined using the Bruker SHELXTL Software Package¹, using the space group P2₁/n (No. 14), with $Z = 4$ for the formula unit, C₆₂H₈₉ClN₄O₂P₂. Non-hydrogen atoms were located from successive difference Fourier map calculations. One solvent THF was found disordered in the adjacent positions in two sets labeled as O(2), C(59), C(60), C(61), C(62) (one set) with 64.042 % occupancies and O(2'), C(59'), C(60'), C(61'), C(62') (another set) (with 35.958% occupancies). Each of these two sets is divided using the PART commands and proper restraints. The atom of P(2) was also found disordered in the adjacent positions in two sets labeled as P(2) and P(2') with occupancies of 30.000% and 70.000%, respectively. In the final cycles of each refinement, all the non-hydrogen atoms were refined in anisotropic displacement parameters. Except for hydrogen atom of H(1) bonded with atom of P(1) that was located from the difference Fourier map and refined with proper restraints, the rest of hydrogen atom positions were calculated and allowed to ride on the carbon to which they are bonded assuming a C–H bond length of m Å (m = 0.930 for Ph–H groups, m = 0.980 for CH groups, m = 0.970 for CH₂ groups, m = 0.960 for CH₃ groups). Hydrogen atom temperature factors were fixed at n (n = 1.2 for CH, CH₂ and Ph–H groups, n = 1.5 for CH₃ groups) times the isotropic temperature factor of the C-atom to which they are bonded. The final anisotropic full-matrix least-squares refinement on F^2 with 699 variables converged at $R1 = 7.75\%$, for the observed data and $wR2 = 21.93\%$ for all data. The goodness-of-fit was 1.014. The largest peak in the final difference electron density

synthesis was $0.476 \text{ e}^-/\text{\AA}^3$ and the largest hole was $-0.328 \text{ e}^-/\text{\AA}^3$ with an RMS deviation of $0.044 \text{ e}^-/\text{\AA}^3$. These largest residues are of no chemical significance. On the basis of the final model, the calculated density was 1.083 g/cm^3 and $F(000)$, 2208 e⁻. The asymmetric unit contains one molecule and two THF solvents with the formula of $\text{C}_{62}\text{H}_{89}\text{ClN}_4\text{O}_2\text{P}_2$. The efforts have been made to resolve as many alerts as possible generated by CheckCIF. The current highest alerts are at level C, which are false alarms.

References

1. (a) Sheldrick, G.M. *SHELXTL-2014, Crystallographic Computing System*; Bruker Analytical X-Ray Instruments: Madison, WI, 2014; (b) Sheldrick, G.M. *A Short History of SHELX*, Acta Cryst. 2008, A64, 112 -122.

Table S2. Sample and crystal data for **6•(THF)₂**

Identification code	6•(THF)₂	
Chemical formula	$\text{C}_{62}\text{H}_{89}\text{ClN}_4\text{O}_2\text{P}_2$	
Formula weight	1019.76 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.120 x 0.200 x 0.420 mm	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	$a = 12.974(3) \text{ Å}$	$\alpha = 90^\circ$
	$b = 31.717(7) \text{ Å}$	$\beta = 95.960(3)^\circ$
	$c = 15.286(3) \text{ Å}$	$\gamma = 90^\circ$
Volume	$6256(2) \text{ Å}^3$	
Z	4	
Density (calculated)	1.083 g/cm^3	
Absorption coefficient	0.154 mm^{-1}	
F(000)	2208	

Table S3. Data collection and structure refinement for **6•(THF)₂**

Theta range for data collection	1.96 to 25.25°	
Index ranges	-15<=h<=15, -38<=k<=38, -18<=l<=18	
Reflections collected	67749	
Independent reflections	11336 [R(int) = 0.0965]	
Max. and min. transmission	0.7454 and 0.6127	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick 2008)	
Refinement method	Full-matrix least-squares on F ²	
Refinement program	SHELXL-2014/6 (Sheldrick, 2014)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	11336 / 217 / 699	
Goodness-of-fit on F²	1.014	
Final R indices	6441 data; I>2σ(I)	R1 = 0.0775, wR2 = 0.1834
	all data	R1 = 0.1367, wR2 = 0.2193
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0819P)^2+5.5929P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.476 and -0.328 eÅ ⁻³	
R.M.S. deviation from mean	0.044 eÅ ⁻³	

Table S4. Bond lengths (Å) for **6•(THF)₂**.

P1-H1	1.278(19)	P1-C1	1.830(3)
P1-P2	2.098(13)	P1-P2'	2.160(6)
P2-C28	1.760(14)	P2'-C28	1.795(7)
N1-C1	1.362(4)	N1-C2	1.377(4)
N1-C16	1.450(4)	N2-C1	1.340(4)
N2-C3	1.377(4)	N2-C4	1.459(4)
N3-C28	1.367(4)	N3-C29	1.385(4)
N3-C43	1.454(4)	N4-C28	1.355(4)
N4-C30	1.391(4)	N4-C31	1.441(4)
C2-C3	1.328(5)	C4-C5	1.387(5)
C4-C9	1.390(5)	C5-C6	1.404(5)
C5-C13	1.504(5)	C6-C7	1.360(6)
C7-C8	1.366(6)	C8-C9	1.384(5)
C9-C10	1.514(6)	C10-C12	1.538(7)
C10-C11	1.507(7)	C13-C15	1.490(7)
C13-C14	1.526(6)	C16-C17	1.402(5)
C16-C21	1.394(5)	C17-C18	1.393(5)
C17-C25	1.494(6)	C18-C19	1.352(7)
C19-C20	1.380(7)	C20-C21	1.376(6)
C21-C22	1.516(6)	C22-C23	1.521(7)
C22-C24	1.520(7)	C25-C27	1.534(6)
C25-C26	1.533(6)	C29-C30	1.320(5)
C31-C32	1.387(5)	C31-C36	1.395(6)
C32-C33	1.405(6)	C32-C40	1.503(6)
C33-C34	1.360(7)	C34-C35	1.358(7)
C35-C36	1.394(6)	C36-C37	1.512(6)
C37-C38	1.513(8)	C37-C39	1.512(8)
C40-C42	1.522(6)	C40-C41	1.510(6)
C43-C48	1.389(5)	C43-C44	1.387(5)
C44-C45	1.394(6)	C44-C52	1.506(6)
C45-C46	1.364(6)	C46-C47	1.357(6)
C47-C48	1.400(5)	C48-C49	1.506(6)
C49-C51	1.531(7)	C49-C50	1.499(7)
C52-C54	1.520(7)	C52-C53	1.515(7)
O1-C55	1.400(12)	O1-C58	1.431(13)
C55-C56	1.493(12)	C56-C57	1.527(12)
C57-C58	1.453(13)	O2-C62	1.340(13)

O2-C59	1.405(15)	C59-C60	1.571(15)
C60-C61	1.465(16)	C61-C62	1.561(13)
O2'-C62'	1.349(14)	O2'-C59'	1.39(2)
C59'-C60'	1.58(2)	C60'-C61'	1.47(2)
C61'-C62'	1.555(15)		

Table 5S. Bond angles (°) for **6•(THF)₂**.

H1-P1-C1	95(2)	H1-P1-P2	114(2)
C1-P1-P2	95.2(4)	H1-P1-P2'	99(2)
C1-P1-P2'	97.87(19)	C28-P2-P1	104.7(5)
C28-P2'-P1	101.1(3)	C1-N1-C2	109.8(3)
C1-N1-C16	126.2(3)	C2-N1-C16	123.8(3)
C1-N2-C3	109.8(3)	C1-N2-C4	127.2(3)
C3-N2-C4	122.8(3)	C28-N3-C29	109.9(3)
C28-N3-C43	126.4(3)	C29-N3-C43	123.0(3)
C28-N4-C30	109.8(3)	C28-N4-C31	126.8(3)
C30-N4-C31	122.7(3)	N1-C1-N2	105.5(3)
N1-C1-P1	130.2(3)	N2-C1-P1	124.2(2)
C3-C2-N1	106.8(3)	C2-C3-N2	108.0(3)
C5-C4-C9	124.3(3)	C5-C4-N2	118.1(3)
C9-C4-N2	117.4(3)	C6-C5-C4	116.2(4)
C6-C5-C13	120.9(4)	C4-C5-C13	122.9(3)
C7-C6-C5	120.5(4)	C8-C7-C6	121.5(4)
C7-C8-C9	121.1(4)	C4-C9-C8	116.3(4)
C4-C9-C10	123.1(3)	C8-C9-C10	120.5(4)
C9-C10-C12	112.1(4)	C9-C10-C11	111.7(4)
C12-C10-C11	110.4(5)	C5-C13-C15	111.8(4)
C5-C13-C14	111.7(4)	C15-C13-C14	111.3(5)
C17-C16-C21	124.5(3)	C17-C16-N1	117.3(3)
C21-C16-N1	118.1(3)	C16-C17-C18	115.1(4)
C16-C17-C25	123.6(3)	C18-C17-C25	121.3(4)
C19-C18-C17	121.6(4)	C18-C19-C20	121.7(4)
C21-C20-C19	120.4(5)	C20-C21-C16	116.6(4)
C20-C21-C22	120.6(4)	C16-C21-C22	122.6(4)
C21-C22-C23	114.2(5)	C21-C22-C24	109.6(4)
C23-C22-C24	110.0(5)	C17-C25-C27	111.6(3)
C17-C25-C26	113.2(4)	C27-C25-C26	108.9(4)
N4-C28-N3	105.0(3)	N4-C28-P2	134.8(5)
N3-C28-P2	118.7(5)	N4-C28-P2'	135.1(3)

N3-C28-P2'	119.0(3)	C30-C29-N3	107.5(3)
C29-C30-N4	107.7(3)	C32-C31-C36	123.8(4)
C32-C31-N4	118.6(3)	C36-C31-N4	117.5(3)
C31-C32-C33	116.1(4)	C31-C32-C40	123.3(4)
C33-C32-C40	120.6(4)	C34-C33-C32	121.1(5)
C35-C34-C33	121.4(5)	C34-C35-C36	120.9(5)
C31-C36-C35	116.6(4)	C31-C36-C37	123.1(4)
C35-C36-C37	120.2(4)	C36-C37-C38	113.3(5)
C36-C37-C39	109.5(5)	C38-C37-C39	112.4(6)
C32-C40-C42	113.0(4)	C32-C40-C41	111.3(4)
C42-C40-C41	109.9(4)	C48-C43-C44	123.6(3)
C48-C43-N3	118.6(3)	C44-C43-N3	117.7(4)
C43-C44-C45	116.3(4)	C43-C44-C52	123.6(4)
C45-C44-C52	120.1(4)	C46-C45-C44	121.9(4)
C45-C46-C47	120.0(4)	C46-C47-C48	121.7(4)
C43-C48-C47	116.4(4)	C43-C48-C49	123.0(3)
C47-C48-C49	120.7(4)	C48-C49-C51	112.4(4)
C48-C49-C50	111.4(4)	C51-C49-C50	109.8(5)
C44-C52-C54	113.3(4)	C44-C52-C53	112.1(4)
C54-C52-C53	109.8(5)	C55-O1-C58	105.9(10)
O1-C55-C56	99.7(11)	C57-C56-C55	112.7(11)
C58-C57-C56	95.5(12)	O1-C58-C57	108.4(11)
C62-O2-C59	99.9(17)	O2-C59-C60	97.3(13)
C61-C60-C59	99.8(15)	C62-C61-C60	100.2(14)
O2-C62-C61	107.1(15)	C62'-O2'-C59'	110(2)
O2'-C59'-C60'	98.1(19)	C61'-C60'-C59'	96(2)
C62'-C61'-C60'	93(2)	O2'-C62'-C61'	105(2)