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SUPPLEMENTARY DATA

Atropisomeric phopshorus-decorated 1-phenyl-3,4-dihydroquinazolin-1-ium NHC precursors

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Table S1. Crystal data and structure refinement for **3.**

Identification code	3
Empirical formula	$C_{32}H_{24}ClN_2O_5PS$
Formula weight	615.01
Temperature/K	300.15
Crystal system	triclinic
Space group	*P*-1
a/Å	9.084(2)
b/Å	12.132(2)
c/Å	13.664(3)
α/°	85.125(6)
β/°	83.809(7)
γ/°	78.065(7)
Volume/Å^3	1461.6(5)
Z	2
ρ_{calc}g/cm^3	1.397
μ/mm^{-1}	0.302
F(000)	636.0
Crystal size/mm^3	0.45 × 0.22 × 0.07
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.438 to 49.928
Index ranges	$-10 \le h \le 10$, $-14 \le k \le 14$, $-16 \le l \le 16$
Reflections collected/independent	13990/5061
Data/restraints/parameters	5061/0/417
Goodness-of-fit on F^2	1.063
Final R indexes [I>=2σ (I)]	R_1 = 0.0564, wR_2 = 0.1343
Final R indexes [all data]	R_1 = 0.0933, wR_2 = 0.1520
Largest diff. peak/hole / e. Å^{-3}	0.44/-0.33

Table S2. Bond Lengths for **3**

Atom	Length/Å	Atom	Length/Å
Cl1–O3	1.301(10)	C2–N2	1.334(4)
Cl1–O4'	1.415(8)	N2–C14'	1.458(4)
Cl1–O2	1.290(15)	N2–C4	1.433(4)
Cl1–O3'	1.272(11)	C14'–C17'	1.399(4)
Cl1–O2'	1.441(11)	C14'–C14	1.387(4)
Cl1–O1'	1.40(2)	C17'–C17	1.404(4)
Cl1–O7	1.330(10)	C22'–C22	1.393(4)
Cl1–O4	1.412(13)	C22'–C18	1.391(4)
S1–P1	1.9546(11)	C22–C21	1.386(5)
P1–C17'	1.832(3)	C21–C20	1.370(6)
P1–C22'	1.812(3)	C20–C19	1.386(6)
P1–C27'	1.822(3)	C27–C27'	1.392(4)
C25–C26	1.366(5)	C27'–C23	1.390(4)
C25–C24	1.378(5)	C17–C16	1.389(5)
C26–C27	1.396(5)	C16–C15	1.381(4)
O1–C4	1.205(4)	C15–C14	1.386(4)
C24–C23	1.388(5)	C4–C4'	1.457(4)
N1–C13'	1.467(4)	C4'–C5	1.401(4)
N1–C2	1.319(4)	C4'–C8'	1.396(4)
N1–C8'	1.425(4)	C5–C6	1.375(5)
C11–C12	1.362(6)	C6–C7	1.383(5)
C11–C10	1.376(7)	C7–C8	1.374(5)
C12–C13	1.391(5)	C8–C8'	1.386(4)
C13–C13'	1.375(5)	C10–C9	1.403(5)
C13'–C9	1.378(5)	C19–C18	1.381(5)

Table S3. Observed angles in **3**

Atom	Angle/°	Atom	Angle/°
O3–Cl1–O4'	105.7(7)	C14–C14'–C17'	122.3(3)
O2–Cl1–O3	107.1(13)	C14'–C17'–P1	123.3(2)
O2–Cl1–O4'	115.6(12)	C14'–C17'–C17	116.9(3)
O3'–Cl1–O3	119.2(13)	C17–C17'–P1	118.9(2)
O3'–Cl1–O4'	105.0(9)	C22–C22'–P1	119.7(2)
O3'–Cl1–O2	104.7(15)	C18–C22'–P1	121.1(2)
O1'–Cl1–O2'	111.1(15)	C18–C22'–C22	119.1(3)
O1'–Cl1–O4	112.3(12)	C21–C22–C22'	120.4(3)
O7–Cl1–O2'	100.2(13)	C20–C21–C22	119.9(4)
O7–Cl1–O1'	114.5(15)	C21–C20–C19	120.4(4)
O7–Cl1–O4	118.2(9)	C27'–C27–C26	119.5(3)
O4–Cl1–O2'	98.3(12)	C27–C27'–P1	119.6(2)
C17'–P1–S1	110.63(10)	C23–C27'–P1	121.2(2)
C22'- P1- S1	112.46(10)	C23–C27'–C27	119.0(3)
C22'–P1–C17'	108.40(13)	C16–C17–C17'	121.0(3)
C22'–P1–C27'	105.79(14)	C15–C16–C17	120.7(3)
C27'–P1–S1	113.21(10)	C16–C15–C14	119.7(3)
C27'–P1–C17'	105.98(13)	C15–C14–C14'	119.5(3)
C26–C25–C24	120.1(4)	O1–C4–N2	119.0(3)
C25–C26–C27	120.9(3)	O1–C4–C4'	127.1(3)
C25–C24–C23	119.9(4)	N2–C4–C4'	113.8(3)
C2–N1–C13'	117.7(3)	C5–C4'–C4	118.8(3)
C2–N1–C8'	120.7(3)	C8'–C4'–C4	121.8(3)
C8'–N1–C13'	121.6(2)	C8'–C4'–C5	119.4(3)
C12–C11–C10	121.1(4)	C6–C5–C4'	119.9(3)
C11–C12–C13	120.3(5)	C5–C6–C7	119.7(4)
C13'–C13–C12	118.4(4)	C8–C7–C6	121.5(3)
C13–C13'–N1	118.1(3)	C7–C8–C8'	119.1(3)
C13–C13'–C9	122.4(3)	C4'–C8'–N1	117.6(3)
C9–C13'–N1	119.5(3)	C8–C8'–N1	122.0(3)
N1–C2–N2	123.1(3)	C8–C8'–C4'	120.3(3)
C2–N2–C14'	119.0(2)	C11–C10–C9	119.8(4)
C2–N2–C4	122.3(3)	C13'–C9–C10	117.9(4)
C4–N2–C14'	118.5(2)	C18–C19–C20	120.0(4)
C17'–C14'–N2	120.4(3)	C19–C18–C22'	120.1(4)
C14–C14'–N2	117.3(3)	C24–C23–C27'	120.7(3)