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Supporting Information
Design, synthesis, photophysical properties and pH-sensing application of the pyrimidine-phthalimide derivatives

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Table S1 Crystallographic Data for **PB**.

Formula sum	C14 H11 N3 O2
Formula weight	253.26 g/mol
Crystal system	triclinic
Space-group	P -1 (2)
Cell parameters	a=8.1726(7) Å b=12.0345(12) Å c=14.2401(12) Å α=110.964(3)° β=103.662(3)° γ=98.181(3)°
Cell ratio	a/b=0.6791 b/c=0.8451 c/a=1.7424
Cell volume	1230.5(2) $Å^3$
Z	4
Calc. density	1.36699 g/cm^3
Meas. density	
Melting point	
RAll	0.1254
RObs	
Pearson code	aP120
Formula type	N2O3P11Q14
Wyckoff sequence	i60

Table S2 Atomic parameters for **PB**.

Atom	Ox.	Wyck.	Site	S.O.F.	x/a	y/b	z/c	U [Å^2]
C1A		2i	1		0.2879(4)	0.7515(3)	0.1079(2)	
C2A		2i	1		0.3241(3)	0.5771(3)	-0.0177(2)	
C3A		2i	1		0.2460(3)	0.5396(3)	0.05398(19)	
C4A		2i	1		0.2273(3)	0.6436(3)	0.1295(2)	
C5A		2i	1		0.1539(4)	0.6370(3)	0.2061(2)	
H5A		2i	1		0.14420	0.70880	0.25900	0.0370
C6A		2i	1		0.0954(3)	0.5217(3)	0.2025(2)	
H6A		2i	1		0.04260	0.51390	0.25330	0.0340
C7A		2i	1		0.1119(4)	0.4171(3)	0.1264(2)	
H7A		2i	1		0.06930	0.33900	0.12550	0.0370
C8A		2i	1		0.1900(4)	0.4245(3)	0.0510(2)	
H8A		2i	1		0.20410	0.35320	-0.00030	0.0320
C9A		2i	1		0.3940(4)	0.7763(3)	-0.03585(19)	
C10A		2i	1		0.5958(4)	0.8599(3)	-0.0909(2)	
C11A		2i	1		0.4712(4)	0.9012(3)	-0.1432(2)	
H11A		2i	1		0.49930	0.94570	-0.18290	0.0340
C12A		2i	1		0.3047(4)	0.8772(3)	-0.1371(2)	
C13A		2i	1		0.7794(4)	0.8843(3)	-0.0939(2)	
H13A		2i	1		0.85470	0.86740	-0.03870	0.0620
H13B		2i	1		0.81920	0.97060	-0.08160	0.0620
H13C		2i	1		0.78410	0.83110	-0.16330	0.0620
C14A		2i	1		0.1626(4)	0.9211(3)	-0.1891(2)	
H14A		2i	1		0.05350	0.85700	-0.21910	0.0610
H14B		2i	1		0.19190	0.93960	-0.24570	0.0610
H14C		2i	1		0.14890	0.99550	-0.13670	0.0610
C1B		2i	1		0.9176(4)	0.3537(3)	0.4149(2)	
C2B		2i	1		0.7271(4)	0.2676(3)	0.4832(2)	
C3B		2i	1		0.6351(3)	0.3322(3)	0.42465(19)	
C4B		2i	1		0.7483(3)	0.3823(3)	0.38329(19)	
C5B		2i	1		0.6971(4)	0.4469(3)	0.3237(2)	
H5B		2i	1		0.77520	0.48180	0.29590	0.0340
C6B		2i	1		0.5283(4)	0.4591(3)	0.3057(2)	
H6B		2i	1		0.48890	0.50200	0.26380	0.0380
C7B		2i	1		0.4147(4)	0.4098(3)	0.3480(2)	
H7B		2i	1		0.29980	0.42060	0.33550	0.0380
C8B		2i	1		0.4675(4)	0.3453(3)	0.4079(2)	
H8B		2i	1		0.39030	0.31110	0.43660	0.0340
C9B		2i	1		1.0235(3)	0.2269(3)	0.5116(2)	
C10B		2i	1		1.1818(4)	0.1898(3)	0.6447(2)	
C11B		2i	1		1.2513(4)	0.1146(3)	0.5742(2)	

H11B	2i	1	1.33390	0.07420	0.59730	0.0340
C12B	2i	1	1.1986(4)	0.0992(3)	0.4699(2)	
C13B	2i	1	1.2316(4)	0.2113(3)	0.7591(2)	
H13D	2i	1	1.27750	0.29960	0.80300	0.0640
H13E	2i	1	1.32090	0.16810	0.77380	0.0640
H13F	2i	1	1.12900	0.18030	0.77540	0.0640
C14B	2i	1	1.2658(4)	0.0195(3)	0.3874(2)	
H14D	2i	1	1.18980	0.00290	0.31690	0.0560
H14E	2i	1	1.26750	-0.05830	0.39480	0.0560
H14F	2i	1	1.38390	0.06170	0.39660	0.0560
N1A	2i	1	0.3478(3)	0.7055(2)	0.02056(16)	
N2A	2i	1	0.2631(3)	0.8114(2)	-0.08278(16)	
N3A	2i	1	0.5585(3)	0.7959(2)	-0.03427(16)	
N1B	2i	1	0.8972(3)	0.2846(2)	0.47528(16)	
N2B	2i	1	1.0810(3)	0.1559(2)	0.43747(17)	
N3B	2i	1	1.0660(3)	0.2479(2)	0.61308(17)	
O1A	2i	1	0.2907(3)	0.8575(2)	0.15381(16)	
O2A	2i	1	0.3588(3)	0.51591(18)	-0.09457(14)	
O1B	2i	1	1.0503(2)	0.3835(2)	0.39670(15)	
O2B	2i	1	0.6735(3)	0.2082(2)	0.52737(16)	

Table S3 Anisotropic displacement parameters for **PB**.

Atom	U11	U22	U33	U12	U13	U23
C1A	0.045(2)	0.023(2)	0.0281(17)	0.0067(16)	0.0192(15)	0.0095(14)
C2A	0.0176(15)	0.0271(18)	0.0209(15)	0.0044(13)	0.0041(12)	0.0111(13)
C3A	0.0179(15)	0.0221(18)	0.0224(15)	0.0052(13)	0.0060(12)	0.0125(13)
C4A	0.0262(16)	0.0237(18)	0.0222(15)	0.0068(14)	0.0093(12)	0.0103(13)
C5A	0.0358(18)	0.034(2)	0.0297(16)	0.0126(16)	0.0173(14)	0.0154(15)
C6A	0.0233(16)	0.047(2)	0.0334(17)	0.0131(15)	0.0169(13)	0.0294(16)
C7A	0.0262(17)	0.033(2)	0.0421(18)	0.0045(15)	0.0097(14)	0.0271(16)
C8A	0.0289(16)	0.0256(18)	0.0287(16)	0.0087(14)	0.0087(13)	0.0149(14)
C9A	0.0324(19)	0.0204(17)	0.0192(15)	0.0009(14)	0.0120(13)	0.0066(13)
C10A	0.0325(17)	0.0186(18)	0.0275(16)	0.0012(14)	0.0143(14)	0.0054(14)
C11A	0.0399(19)	0.0205(18)	0.0262(16)	0.0005(15)	0.0142(14)	0.0111(14)
C12A	0.0344(18)	0.0194(17)	0.0196(15)	0.0018(14)	0.0079(13)	0.0064(13)
C13A	0.038(2)	0.033(2)	0.055(2)	0.0021(16)	0.0263(16)	0.0161(17)
C14A	0.045(2)	0.043(2)	0.0347(18)	0.0064(17)	0.0089(15)	0.0216(17)
C1B	0.0277(17)	0.0251(18)	0.0225(15)	0.0080(14)	0.0110(13)	0.0094(14)
C2B	0.0281(17)	0.0322(19)	0.0277(16)	0.0097(15)	0.0099(13)	0.0142(15)
C3B	0.0229(16)	0.0212(17)	0.0194(14)	0.0030(13)	0.0057(12)	0.0071(13)
C4B	0.0194(15)	0.0255(18)	0.0205(14)	0.0042(13)	0.0080(12)	0.0094(13)
C5B	0.0240(17)	0.036(2)	0.0286(16)	0.0026(15)	0.0099(13)	0.0175(15)
C6B	0.0264(17)	0.043(2)	0.0340(17)	0.0107(15)	0.0092(14)	0.0245(16)
C7B	0.0234(16)	0.042(2)	0.0341(17)	0.0120(15)	0.0091(13)	0.0190(16)
C8B	0.0230(16)	0.038(2)	0.0313(16)	0.0058(15)	0.0110(13)	0.0200(15)
C9B	0.0214(16)	0.0226(18)	0.0312(17)	0.0038(14)	0.0089(13)	0.0125(14)
C10B	0.0279(17)	0.0240(18)	0.0270(16)	0.0048(15)	0.0038(13)	0.0111(14)
C11B	0.0262(17)	0.0271(19)	0.0335(17)	0.0129(14)	0.0057(14)	0.0143(14)
C12B	0.0240(16)	0.0231(18)	0.0339(17)	0.0053(14)	0.0092(13)	0.0100(14)
C13B	0.055(2)	0.039(2)	0.0303(18)	0.0170(18)	0.0052(16)	0.0136(16)
C14B	0.043(2)	0.031(2)	0.0389(18)	0.0170(17)	0.0177(15)	0.0098(15)
N1A	0.0381(15)	0.0183(15)	0.0249(13)	0.0056(12)	0.0165(11)	0.0102(11)
N2A	0.0315(14)	0.0228(15)	0.0235(13)	0.0007(12)	0.0098(11)	0.0092(12)
N3A	0.0298(15)	0.0223(15)	0.0292(13)	0.0035(12)	0.0135(11)	0.0098(11)
N1B	0.0231(14)	0.0322(16)	0.0299(13)	0.0123(12)	0.0121(11)	0.0187(12)
N2B	0.0265(14)	0.0257(15)	0.0288(13)	0.0089(12)	0.0086(11)	0.0116(12)
N3B	0.0307(14)	0.0257(15)	0.0244(13)	0.0078(12)	0.0091(11)	0.0109(11)
O1A	0.100(2)	0.0214(14)	0.0478(14)	0.0152(14)	0.0504(14)	0.0114(11)
O2A	0.0429(13)	0.0270(12)	0.0280(11)	0.0104(10)	0.0202(10)	0.0112(9)
O1B	0.0256(12)	0.0465(15)	0.0445(12)	0.0114(11)	0.0182(10)	0.0264(11)
O2B	0.0341(13)	0.0535(16)	0.0502(13)	0.0133(11)	0.0172(10)	0.0393(12)

Table S4 Crystallographic Data for **NPB**.

Formula sum	C40 H45 N5 O4

Formula weight	659.81 g/mol
Crystal system	monoclinic
Space-group	P 1 21/n 1 (14)
Cell parameters	a=15.7201(16) Å b=8.3942(6) Å c=26.601(2) Å β=99.639(3)°
Cell ratio	a/b=1.8727 b/c=0.3156 c/a=1.6922
Cell volume	3460.65(50) $Å^3$
Z	4
Calc. density	1.26632 g/cm^3
Meas. density	
Melting point	
RAll	0.1269
RObs	
Pearson code	mP480
Formula type	N4O5P40Q61
Wyckoff sequence	e120

Table S5 Atomic parameters for **NPB**.

Atom	Ox.	Wyck.	Site	S.O.F.	x/a	y/b	z/c	U [Å²]
C1		4e	1		0.9363(2)	0.1781(3)	0.23730(12)	
C2		4e	1		1.0538(2)	0.3470(3)	0.25807(11)	
C3		4e	1		1.08675(19)	0.1808(3)	0.25805(10)	
C4		4e	1		1.01695(19)	0.0807(3)	0.24575(11)	
C5		4e	1		1.0280(2)	-0.0826(3)	0.24382(13)	
H5		4e	1		0.98020	-0.15240	0.23530	0.0490
C6		4e	1		1.1117(2)	-0.1401(4)	0.25482(12)	
H6		4e	1		1.12130	-0.25170	0.25390	0.0490
C7		4e	1		1.1816(2)	-0.0390(3)	0.26714(12)	
H7		4e	1		1.23820	-0.08190	0.27430	0.0440
C8		4e	1		1.1697(2)	0.1240(3)	0.26905(11)	
H8		4e	1		1.21730	0.19420	0.27770	0.0400
C9		4e	1		0.90816(19)	0.4728(3)	0.24561(11)	
C10		4e	1		0.85290(18)	0.6576(3)	0.29291(11)	
C11		4e	1		0.81245(18)	0.7259(3)	0.24781(11)	
H11		4e	1		0.77690	0.81710	0.24860	0.0330
C12		4e	1		0.82407(18)	0.6607(3)	0.20141(11)	
C13		4e	1		0.84841(19)	0.7277(3)	0.34272(11)	
H13		4e	1		0.80670	0.80810	0.34510	0.0350
C14		4e	1		0.90117(19)	0.6822(3)	0.38501(11)	
H14		4e	1		0.93780	0.59500	0.38060	0.0350
C15		4e	1		0.94441(19)	0.8671(3)	0.53770(11)	
C16		4e	1		0.87345(19)	0.9190(3)	0.50243(11)	
H16		4e	1		0.83540	0.99600	0.51250	0.0360
C17		4e	1		0.85787(19)	0.8604(3)	0.45328(11)	
H17		4e	1		0.80970	0.89930	0.43020	0.0360
C18		4e	1		0.91133(19)	0.7447(3)	0.43650(11)	
C19		4e	1		0.9806(2)	0.6916(3)	0.47252(11)	
H19		4e	1		1.01760	0.61210	0.46270	0.0370
C20		4e	1		0.9974(2)	0.7496(3)	0.52167(11)	
H20		4e	1		1.04520	0.70970	0.54490	0.0380
C21		4e	1		0.9077(2)	1.0481(4)	0.60336(13)	
H21A		4e	1		0.90320	1.13870	0.57980	0.0680
H21B		4e	1		0.93310	1.08360	0.63770	0.0680
H21C		4e	1		0.85000	1.00440	0.60390	0.0680
C22		4e	1		1.0369(2)	0.8710(4)	0.62216(12)	
H22A		4e	1		1.02880	0.75910	0.63070	0.0650
H22B		4e	1		1.04380	0.93550	0.65330	0.0650
H22C		4e	1		1.08860	0.88110	0.60630	0.0650
C23		4e	1		0.78813(19)	0.7342(3)	0.15281(11)	

H23	4e	1		0.74990	0.82180	0.15300	0.0350
C24	4e	1		0.80630(18)	0.6842(3)	0.10801(11)	
H24	4e	1		0.84040	0.59040	0.10930	0.0340
C25	4e	1		0.74036(19)	0.8845(3)	-0.04212(11)	
C26	4e	1		0.70752(19)	0.9504(3)	-0.00060(11)	
H26	4e	1		0.67080	1.04090	-0.00600	0.0370
C27	4e	1		0.72742(19)	0.8865(3)	0.04753(11)	
H27	4e	1		0.70410	0.93410	0.07460	0.0350
C28	4e	1		0.78115(18)	0.7534(3)	0.0577(1)	
C29	4e	1		0.8134(2)	0.6889(3)	0.01641(11)	
H29	4e	1		0.85000	0.59830	0.02190	0.0390
C30	4e	1		0.7944(2)	0.7515(3)	-0.03202(11)	
H30	4e	1		0.81820	0.70380	-0.05890	0.0410
C31	4e	1		0.6583(3)	1.0743(4)	-0.10109(13)	
H31A	4e	1		0.60130	1.03330	-0.09750	0.0830
H31B	4e	1		0.65700	1.11290	-0.13600	0.0830
H31C	4e	1		0.67380	1.16210	-0.07700	0.0830
C32	4e	1		0.7499(3)	0.8721(4)	-0.13326(12)	
H32A	4e	1		0.81310	0.86850	-0.12760	0.0750
H32B	4e	1		0.72910	0.93250	-0.16440	0.0750
H32C	4e	1		0.72690	0.76340	-0.13690	0.0750
N1	4e	1		0.96439(15)	0.3369(3)	0.24535(9)	
N2	4e	1		0.87409(15)	0.5285(3)	0.20049(9)	
N3	4e	1		0.90197(15)	0.5248(3)	0.29183(9)	
N4	4e	1		0.96171(18)	0.9265(3)	0.58656(9)	
N5	4e	1		0.72125(19)	0.9488(3)	-0.09039(9)	
O1	4e	1		0.86281(15)	0.1367(3)	0.22656(11)	
O2	4e	1		1.09456(14)	0.4689(2)	0.26686(9)	
O3A	4e	1	0.671	0.1473(4)	0.4946(6)	0.1302(2)	
C33A	4e	1	0.671	0.0601(6)	0.521(1)	0.1282(4)	
H33A	4e	1	0.671	0.04360	0.49320	0.16140	0.1330
H33B	4e	1	0.671	0.02700	0.45170	0.10180	0.1330
C34A	4e	1	0.671	0.0383(4)	0.6893(8)	0.1161(3)	
H34A	4e	1	0.671	0.00750	0.73740	0.14190	0.1000
H34B	4e	1	0.671	0.00240	0.70010	0.08200	0.1000
C35A	4e	1	0.671	0.1252(4)	0.7641(7)	0.1175(3)	
H35A	4e	1	0.671	0.12330	0.84620	0.09070	0.0920
H35B	4e	1	0.671	0.14560	0.81390	0.15110	0.0920
C36A	4e	1	0.671	0.1796(6)	0.6358(12)	0.1088(5)	
H36A	4e	1	0.671	0.23980	0.65710	0.12530	0.1240
H36B	4e	1	0.671	0.17870	0.62150	0.07170	0.1240
O3B	4e	1	0.671	0.8914(4)	0.3240(6)	0.06026(18)	

C33B	4e	1	0.671	0.8721(6)	0.2279(11)	0.0998(3)	
H33C	4e	1	0.671	0.81350	0.18210	0.09060	0.0790
H33D	4e	1	0.671	0.87440	0.29100	0.13140	0.0790
C34B	4e	1	0.671	0.9383(5)	0.0984(8)	0.1073(2)	
H34C	4e	1	0.671	0.91350	-0.00180	0.11810	0.0780
H34D	4e	1	0.671	0.98830	0.12920	0.13330	0.0780
C35B	4e	1	0.671	0.9640(9)	0.0804(15)	0.0560(3)	
H35C	4e	1	0.671	1.02760	0.08160	0.05860	0.0990
H35D	4e	1	0.671	0.94130	-0.02000	0.03940	0.0990
C36B	4e	1	0.671	0.9245(6)	0.2211(9)	0.0272(3)	
H36C	4e	1	0.671	0.96840	0.27720	0.01120	0.1200
H36D	4e	1	0.671	0.87760	0.18590	-0.00010	0.1200
O3Z	4e	1	0.329	0.1846(11)	0.595(2)	0.1166(7)	0.113(4)
C33Z	4e	1	0.329	0.1287(12)	0.557(3)	0.1504(6)	0.105(4)
H33G	4e	1	0.329	0.14240	0.62330	0.18160	0.1260
H33H	4e	1	0.329	0.13490	0.44390	0.16040	0.1260
C34Z	4e	1	0.329	0.0397(12)	0.589(3)	0.1247(7)	0.115(5)
H34G	4e	1	0.329	0.01640	0.68720	0.13810	0.1380
H34H	4e	1	0.329	0.00100	0.49870	0.12860	0.1380
C35Z	4e	1	0.329	0.0506(9)	0.610(2)	0.0698(5)	0.093(4)
H35G	4e	1	0.329	0.04550	0.50680	0.05160	0.1120
H35H	4e	1	0.329	0.00680	0.68460	0.05180	0.1120
C36Z	4e	1	0.329	0.1375(10)	0.6757(19)	0.0731(6)	0.092(4)
H36G	4e	1	0.329	0.16170	0.65210	0.04180	0.1110
H36H	4e	1	0.329	0.13770	0.79240	0.07850	0.1110
O3Y	4e	1	0.329	0.9635(8)	0.1711(14)	0.1352(4)	0.107(4)
C33Y	4e	1	0.329	0.8764(12)	0.204(4)	0.1116(7)	0.082(5)
H33E	4e	1	0.329	0.85550	0.30380	0.12520	0.0980
H33F	4e	1	0.329	0.83760	0.11570	0.11770	0.0980
C34Y	4e	1	0.329	0.8798(11)	0.220(2)	0.0565(6)	0.083(4)
H34E	4e	1	0.329	0.90160	0.32560	0.04820	0.0990
H34F	4e	1	0.329	0.82280	0.20010	0.03520	0.0990
C35Y	4e	1	0.329	0.9439(17)	0.088(4)	0.0507(7)	0.082(5)
H35E	4e	1	0.329	0.91360	-0.01040	0.03710	0.0980
H35F	4e	1	0.329	0.98380	0.12110	0.02750	0.0980
C36Y	4e	1	0.329	0.9911(12)	0.062(2)	0.1029(6)	0.115(5)
H36E	4e	1	0.329	0.98030	-0.04760	0.11430	0.1380
H36F	4e	1	0.329	1.05390	0.07410	0.10340	0.1380

Table S6 Anisotropic displacement parameters for **NPB**.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.0288(19)	0.0291(17)	0.046(2)	-0.0033(14)	0.0073(15)	-0.0050(14)
C2	0.0361(18)	0.0212(15)	0.0273(17)	0.0014(13)	0.0005(13)	0.0011(12)
C3	0.0310(18)	0.0209(14)	0.0234(15)	0.0012(12)	0.0020(12)	0.0007(12)
C4	0.0303(18)	0.0227(15)	0.0335(17)	-0.0011(12)	0.0075(14)	-0.0018(13)
C5	0.039(2)	0.0249(16)	0.060(2)	-0.0069(14)	0.0136(17)	-0.0065(15)
C6	0.049(2)	0.0236(16)	0.050(2)	0.0059(15)	0.0125(17)	-0.0013(14)
C7	0.0347(19)	0.0298(17)	0.0439(19)	0.0072(14)	0.0053(15)	0.0004(14)
C8	0.0318(19)	0.0274(17)	0.0410(19)	-0.0025(13)	0.0056(14)	-0.0004(13)
C9	0.0328(18)	0.0234(15)	0.0312(17)	0.0029(13)	0.0028(14)	-0.0008(13)
C10	0.0260(17)	0.0254(15)	0.0293(16)	-0.0009(13)	0.0068(13)	-0.0003(13)
C11	0.0219(16)	0.0267(15)	0.0340(17)	0.0040(12)	0.0058(13)	-0.0007(13)
C12	0.0215(16)	0.0266(15)	0.0295(16)	-0.0019(12)	0.0019(12)	-0.0005(13)
C13	0.0289(17)	0.0291(16)	0.0312(17)	0.0033(13)	0.0081(13)	0.0000(13)
C14	0.0333(18)	0.0221(15)	0.0325(17)	0.0020(13)	0.0100(14)	0.0002(13)
C15	0.0327(18)	0.0260(15)	0.0256(16)	-0.0032(13)	0.0076(13)	0.0004(12)
C16	0.0303(18)	0.0304(16)	0.0316(17)	0.0018(13)	0.0083(14)	-0.0025(13)
C17	0.0264(17)	0.0303(16)	0.0319(17)	0.0022(13)	0.0040(13)	0.0029(13)
C18	0.0324(18)	0.0195(14)	0.0302(16)	-0.0029(13)	0.0087(13)	0.0021(12)
C19	0.0329(18)	0.0277(16)	0.0329(17)	0.0055(13)	0.0091(14)	0.0019(13)
C20	0.0330(18)	0.0294(16)	0.0310(17)	0.0021(13)	0.0018(14)	0.0040(13)
C21	0.045(2)	0.054(2)	0.039(2)	-0.0036(17)	0.0150(17)	-0.0142(16)
C22	0.052(2)	0.048(2)	0.0290(18)	-0.0029(17)	0.0016(16)	-0.0006(15)
C23	0.0252(17)	0.0291(16)	0.0315(17)	0.0036(13)	-0.0002(13)	-0.0007(13)
C24	0.0232(16)	0.0270(15)	0.0326(17)	-0.0021(12)	-0.0012(13)	-0.0030(13)
C25	0.0301(18)	0.0296(16)	0.0296(17)	-0.0043(13)	0.0014(13)	-0.0036(13)
C26	0.0299(18)	0.0292(16)	0.0332(18)	0.0041(13)	0.0025(14)	-0.0013(13)
C27	0.0286(17)	0.0328(16)	0.0266(16)	0.0016(13)	0.0034(13)	-0.0039(13)
C28	0.0219(16)	0.0281(15)	0.0269(16)	-0.0014(12)	0.0002(12)	-0.0023(12)
C29	0.0332(19)	0.0295(16)	0.0348(18)	0.0066(13)	0.0024(14)	-0.0034(14)
C30	0.0380(19)	0.0335(17)	0.0305(17)	0.0028(14)	0.0065(14)	-0.0042(14)
C31	0.063(3)	0.063(2)	0.040(2)	0.019(2)	0.0116(19)	0.0169(18)
C32	0.070(3)	0.054(2)	0.0277(18)	0.0100(19)	0.0113(17)	0.0014(16)
N1	0.0278(14)	0.0221(12)	0.0302(14)	0.0028(10)	0.0008(11)	-0.0023(10)
N2	0.0297(15)	0.0269(13)	0.0288(14)	0.0028(11)	0.0017(11)	-0.0012(11)
N3	0.0317(15)	0.0259(13)	0.0285(14)	0.0032(11)	0.0024(11)	-0.0004(11)
N4	0.0432(18)	0.0399(15)	0.0304(15)	0.0021(12)	0.0052(13)	-0.0084(12)
N5	0.0542(19)	0.0425(16)	0.0280(15)	0.0144(14)	0.0091(13)	0.0023(12)
O1	0.0290(15)	0.0405(14)	0.107(2)	-0.0018(11)	0.0097(14)	-0.0107(14)
O2	0.0423(14)	0.0227(11)	0.0629(16)	-0.0028(10)	-0.0062(12)	-0.0039(11)
O3A	0.115(4)	0.070(3)	0.111(4)	0.034(3)	0.014(3)	0.024(3)

C33A	0.079(5)	0.093(6)	0.158(6)	-0.018(5)	0.014(5)	0.034(5)
C34A	0.055(4)	0.081(5)	0.115(5)	0.009(4)	0.022(4)	0.003(4)
C35A	0.082(5)	0.059(4)	0.095(5)	-0.011(3)	0.036(4)	-0.013(3)
C36A	0.057(4)	0.113(7)	0.142(7)	0.015(5)	0.023(5)	0.035(6)
O3B	0.120(4)	0.056(3)	0.075(3)	0.026(3)	0.009(3)	0.005(2)
C33B	0.077(4)	0.049(4)	0.070(5)	0.008(3)	0.006(4)	-0.012(4)
C34B	0.074(4)	0.058(3)	0.067(4)	0.007(3)	0.020(3)	-0.007(3)
C35B	0.098(7)	0.073(5)	0.080(5)	0.017(5)	0.024(5)	-0.010(4)
C36B	0.145(7)	0.087(5)	0.073(5)	0.021(5)	0.035(5)	0.007(4)

Table S7 Cartesian coordinates for the optimized structure of **PB**. (Total energy = -850.12393116 Hartree)

Current cartesian coordinates R N= 90

-5.78584618E+00 2.22389693E+00 -6.46717856E-01 -3.25327095E+00 2.05990091E+00

-9.19412008E-01 -2.27473089E+00 -2.19469785E-01 -3.76907805E-01 -3.44832814E+00

-2.28916667E+00 5.23453515E-01 -5.98692697E+00 -2.12622214E+00 6.46060742E-01

-7.23045482E+00 1.20173527E-01 1.95189058E-02 -6.95088594E+00 4.75869168E+00

-1.19352359E+00 -7.38317688E+00 -4.42641960E+00 1.57416672E+00 2.91755384E-01

-2.43817110E-01 -1.56105172E-02 1.66841103E+00 2.03046058E+00 6.90601228E-01

4.35774229E+00 1.22634796E+00 4.16219343E-01 4.49858422E+00 -1.30211645E+00

-3.04798312E-01 1.92185499E+00 -2.35684668E+00 -7.04446174E-01 6.46931839E+00

2.68305889E+00 8.48166555E-01 8.80479625E+00 1.50020146E+00 4.90553024E-01

8.95882930E+00 -1.08153127E+00 -1.08610403E-01 6.79333707E+00 -2.48846886E+00

-6.44119691E-01 1.31260646E+00 -4.40834288E+00 -1.55970918E+00 8.46734501E-01

4.12330967E+00 1.20097635E+00 -9.25742489E+00 2.48198692E-01 1.05585405E-01

-8.96089108E+00 4.77324429E+00 -7.68333241E-01 -6.69112370E+00 5.11345199E+00

-3.21056000E+00 -6.02216962E+00 6.28574156E+00 -1.73134818E-01 -9.38640427E+00

-4.01629398E+00 1.78532549E+00 -6.59039848E+00 -4.98704322E+00 3.38931560E+00

-7.14751848E+00 -6.01584312E+00 2.77962576E-01 6.29751670E+00 4.69205410E+00

1.15324351E+00 1.05144859E+01 2.57276423E+00 7.27739770E-01 1.07858263E+01

-1.90636042E+00 -4.75542835E-01 6.88716869E+00 -4.41860586E+00 -1.29773185E+00

Table S8 Cartesian coordinates for the optimized structure of **NPB**. (Total energy = -1660.63861880 Hartree)

Current cartesian coordinates R N= 204

2.29238639E+00 -1.51779116E+00 -4.67373002E-02 2.26712196E+00 1.06822862E+00
-8.88753164E-02 7.05212513E-06 2.18128008E+00 3.74100899E-05 -2.26718361E+00
1.06831621E+00 8.89494558E-02 -2.29254866E+00 -1.51770256E+00 4.68808078E-02
-1.02551443E-04 -2.85802159E+00 1.29350134E-04 4.71884825E+00 -2.80946959E+00
-7.58133755E-02 -4.71904888E+00 -2.80931884E+00 7.59848527E-02 5.27579023E-05
4.87381031E+00 4.42834926E-05 1.21530641E+00 6.37818513E+00 1.86154354E+00
7.30805099E-01 9.04335660E+00 1.10339734E+00 -7.30358567E-01 9.04337996E+00
-1.10347613E+00 -1.21507626E+00 6.37822862E+00 -1.86153451E+00 -2.36840062E+00
5.59296892E+00 -3.73109246E+00 2.36858869E+00 5.59290782E+00 3.73112684E+00
1.48266028E+00 1.12827875E+01 2.24895459E+00 7.30271996E-01 1.35589012E+01
1.10803977E+00 -7.29094972E-01 1.35589263E+01 -1.10848771E+00 -1.48186085E+00
1.12828416E+01 -2.24920935E+00 6.96363679E+00 -1.57293216E+00 -6.24154589E-02
-6.96381757E+00 -1.57275262E+00 6.24670075E-02 9.48750037E+00 -2.66328408E+00
-8.68122929E-02 -9.48769513E+00 -2.66306879E+00 8.67750066E-02 1.16074642E+01
-1.04311589E+00 -3.41691534E-02 1.40695963E+01 -1.95597000E+00 -5.36455419E-02
1.45522650E+01 -4.59129466E+00 -1.28241561E-01 1.24289274E+01 -6.23530350E+00
-1.83009868E-01 9.98360997E+00 -5.28679451E+00 -1.62893298E-01 -1.16076319E+01
-1.04285228E+00 3.46647343E-02 -1.40697855E+01 -1.95566786E+00 5.41200882E-02
-1.45525038E+01 -4.59099652E+00 1.28035179E-01 -1.24291891E+01 -6.23505232E+00
1.82351585E-01 -9.98385338E+00 -5.28658428E+00 1.62307322E-01 1.70006734E+01
-5.53151730E+00 -1.47435684E-01 1.74458848E+01 -8.25749705E+00 -2.18440105E-01
1.91514656E+01 -3.79744186E+00 -9.21988001E-02 -1.70009245E+01 -5.53118212E+00
1.47077817E-01 -1.91516949E+01 -3.79703683E+00 9.34694767E-02 -1.74461917E+01
-8.25716103E+00 2.17773386E-01 -1.28745101E-04 -4.90720423E+00 2.21258397E-04
4.63430938E+00 -4.86177589E+00 -9.76774603E-02 -4.63453276E+00 -4.86162422E+00
9.80445330E-02 2.61061610E+00 1.12617992E+01 3.95946267E+00 1.28518362E+00

1.53449448E+01 1.94864076E+00 -1.28371726E+00 1.53449886E+01 -1.94924026E+00
-2.60982345E+00 1.12619075E+01 -3.95971353E+00 6.87000253E+00 4.81380584E-01
-2.29363033E-02 -6.87015591E+00 4.81558013E-01 2.30440472E-02 1.12991541E+01
9.85924974E-01 2.63867116E-02 1.56193843E+01 -6.22053629E-01 -9.77639116E-03
1.26993367E+01 -8.26214217E+00 -2.42302225E-01 8.42199160E+00 -6.61593944E+00
-2.09113478E-01 -1.12993175E+01 9.86201395E-01 -2.54313692E-02 -1.56195370E+01
-6.21689711E-01 1.07394112E-02 -1.26996195E+01 -8.26189949E+00 2.41291402E-01
-8.42226912E+00 -6.61578411E+00 2.08144867E-01 1.94767402E+01 -8.61128847E+00
-2.20092793E-01 1.66424827E+01 -9.12588110E+00 -1.92515754E+00 1.66292568E+01
-9.21495196E+00 1.43343687E+00 2.09009661E+01 -4.88728684E+00 -1.19422437E-01
1.91506805E+01 -2.62477028E+00 1.62161773E+00 1.91584796E+01 -2.52888739E+00
-1.73619107E+00 -2.09012173E+01 -4.88685597E+00 1.20365227E-01 -1.91512677E+01
-2.62327419E+00 -1.61959045E+00 -1.91583345E+01 -2.52952165E+00 1.73827684E+00
-1.94770476E+01 -8.61095913E+00 2.18150078E-01 -1.66437547E+01 -9.12574007E+00
1.92486805E+00 -1.66286399E+01 -9.21444108E+00 -1.43372608E+00

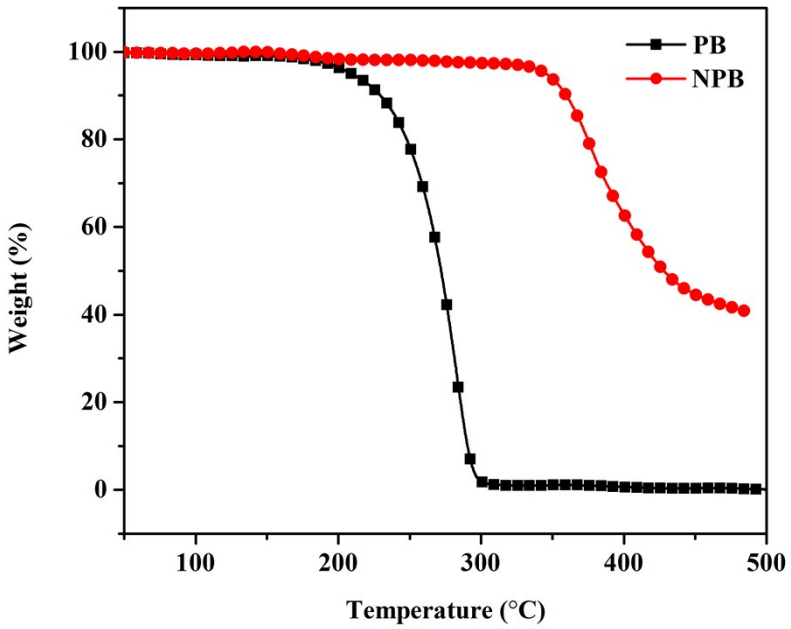

Fig. S1. Thermogravimetric analysis of **PB** and **NPB** with a heating rate of 10 °C min $^{-1}$ under N_2 atmosphere.

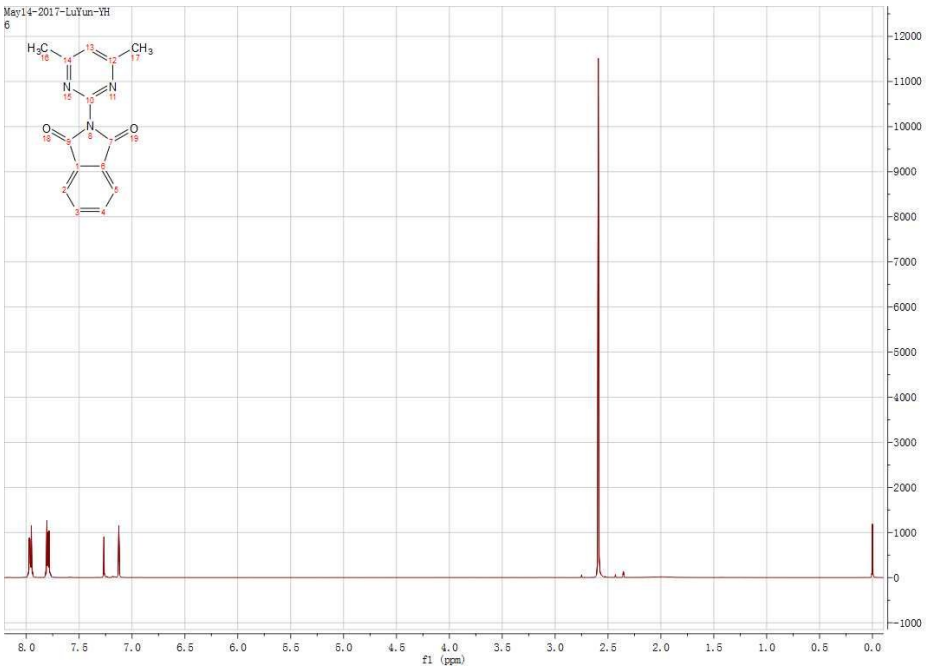

Fig. S2. The ^{1}H NMR spectrum of **PB**.

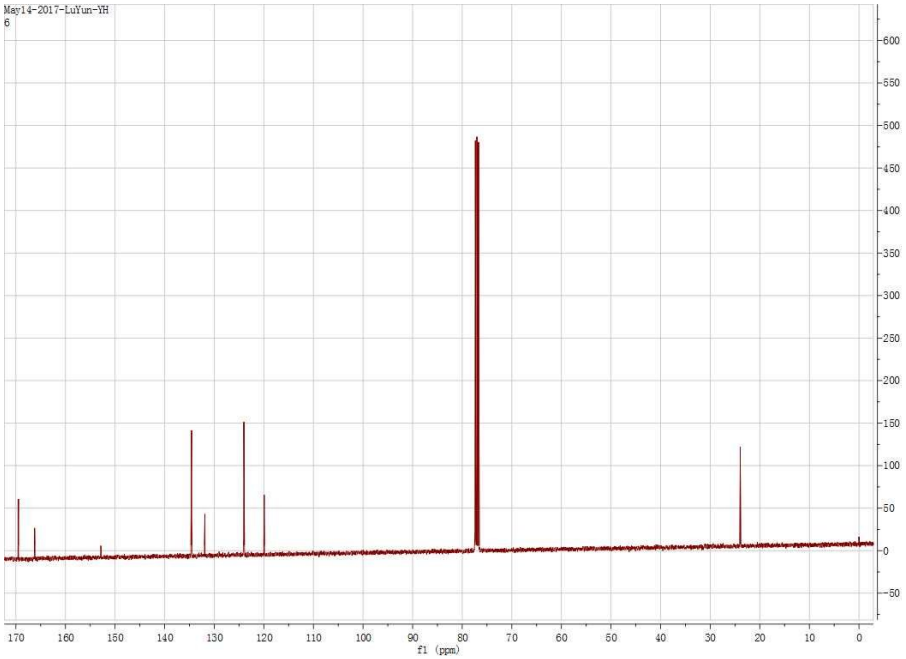

Fig. S3. The ^{13}C NMR spectrum of **PB**.

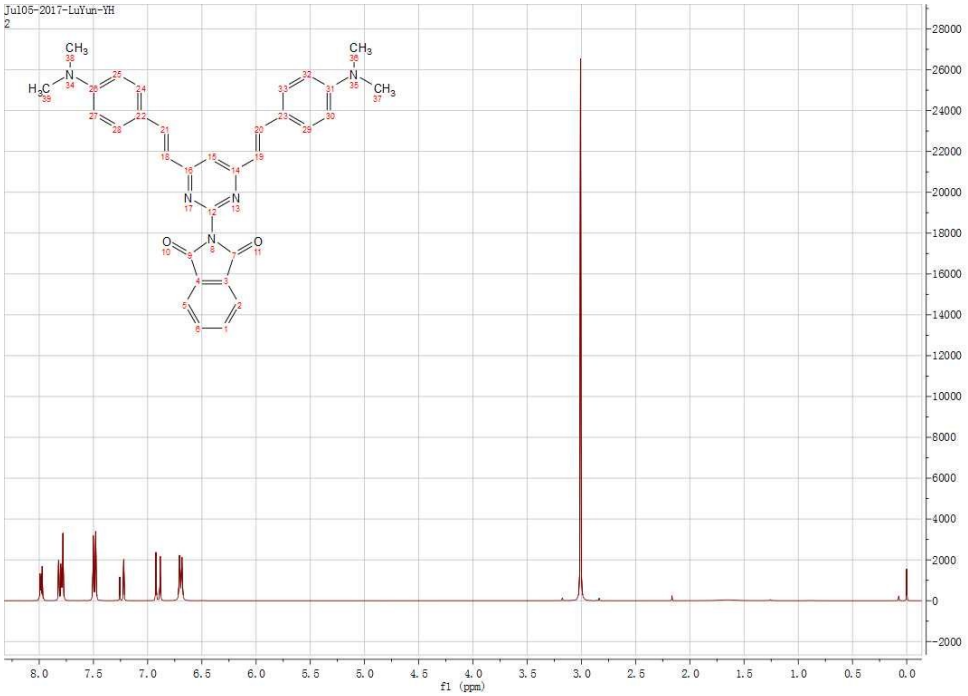

Fig. S4. The ^{1}H NMR spectrum of **NPB**.

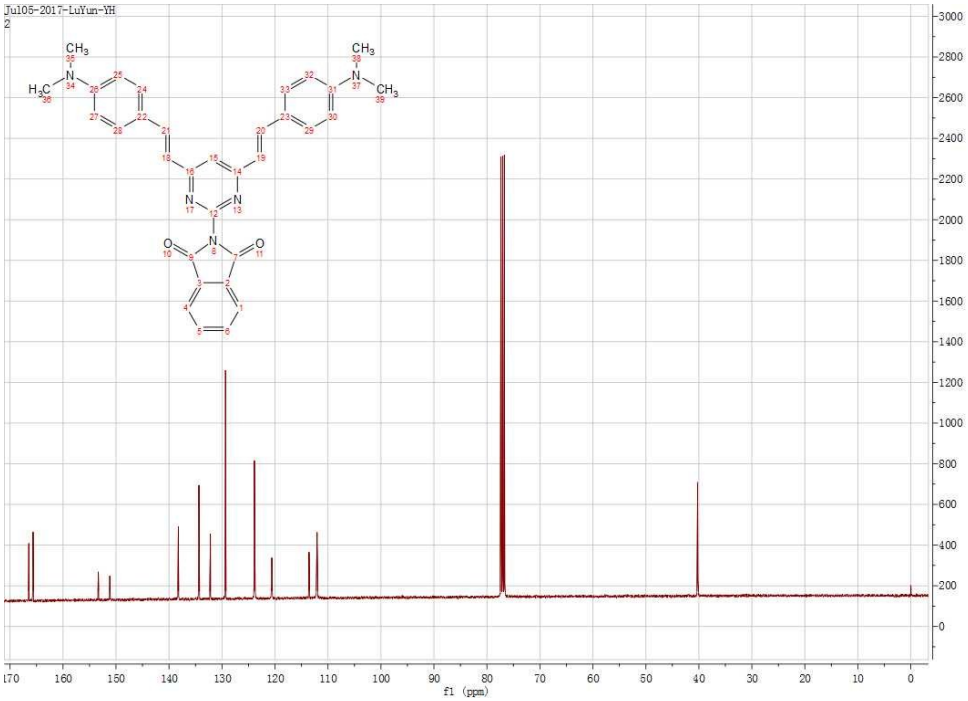

Fig. S5. The ^{13}C NMR spectrum of **NPB**.