Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for

Synthesis, Characterization, and Cure Chemistry of High Performance Phosphate Cyanate Ester Resins

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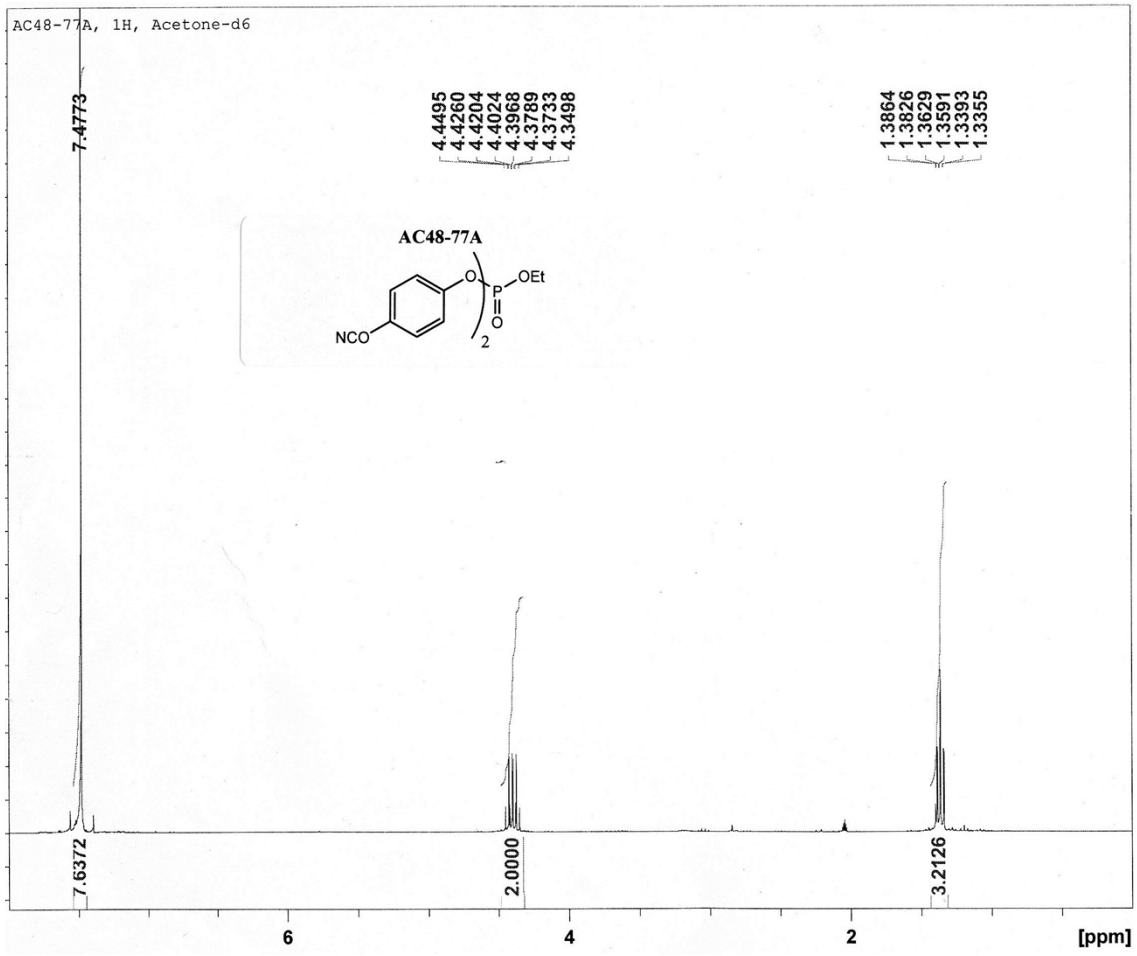

Figure S1. ^{1}H NMR spectrum of PhosCy

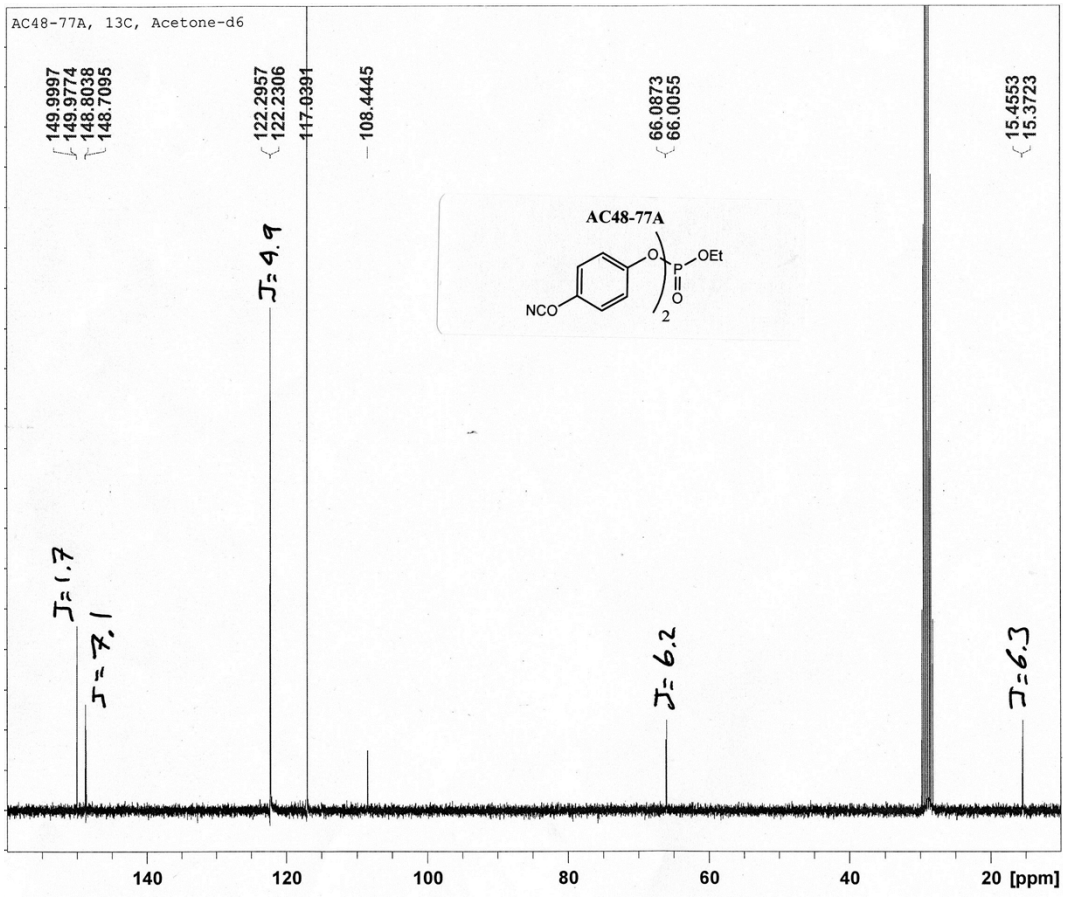

Figure S2. ^{13}C NMR spectrum of PhosCy

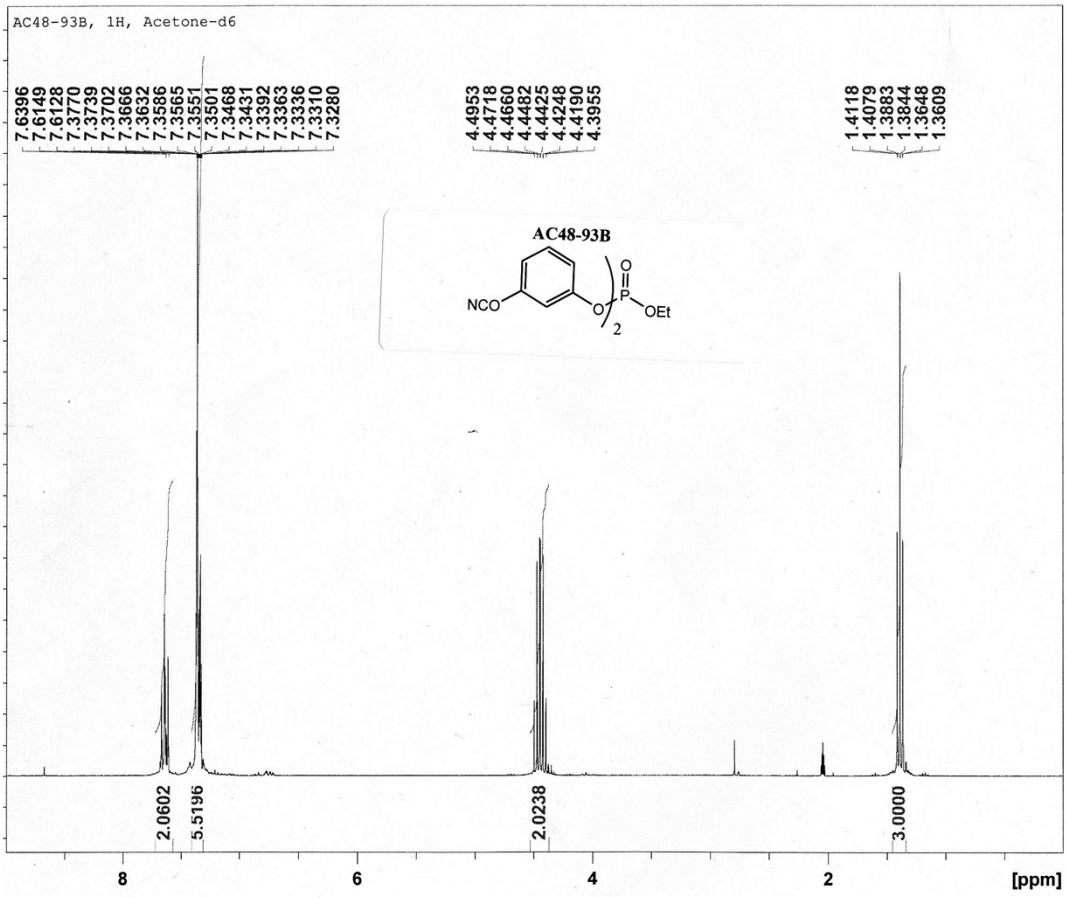

Figure S3. ^{1}H NMR spectrum of MPhosCy

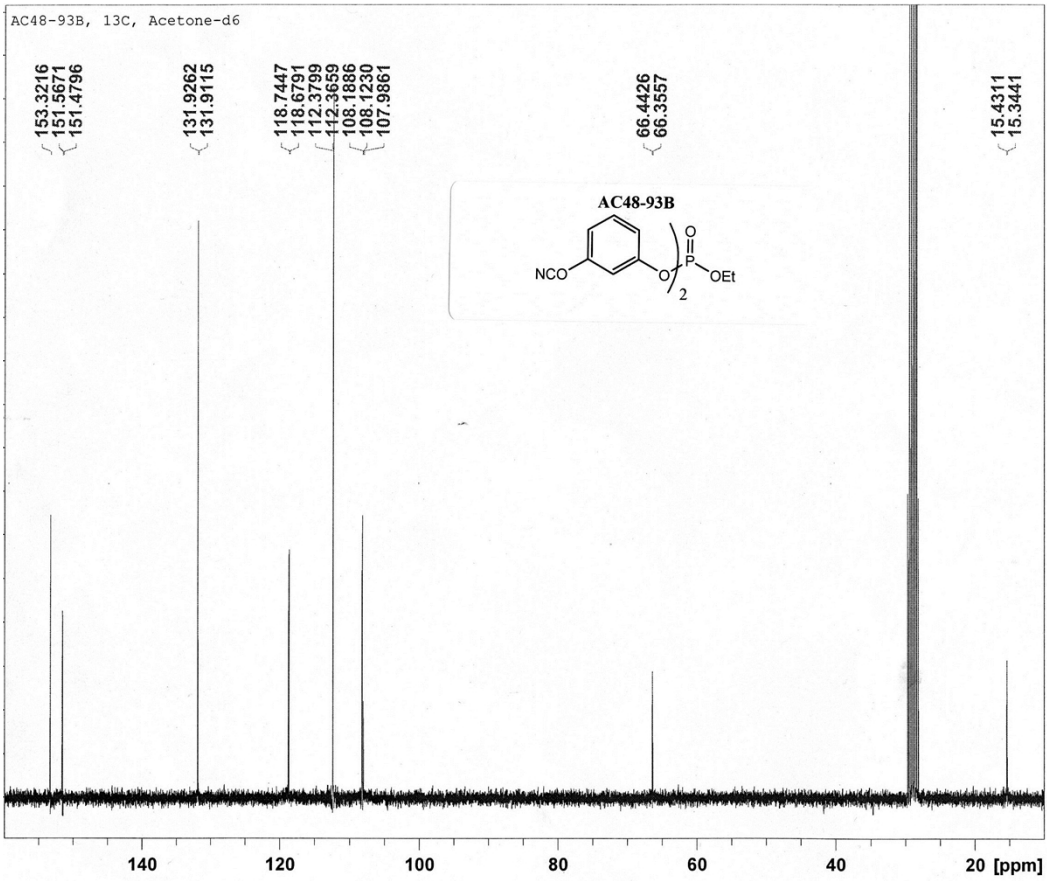

Figure S4. ^{13}C NMR spectrum of MPhosCy

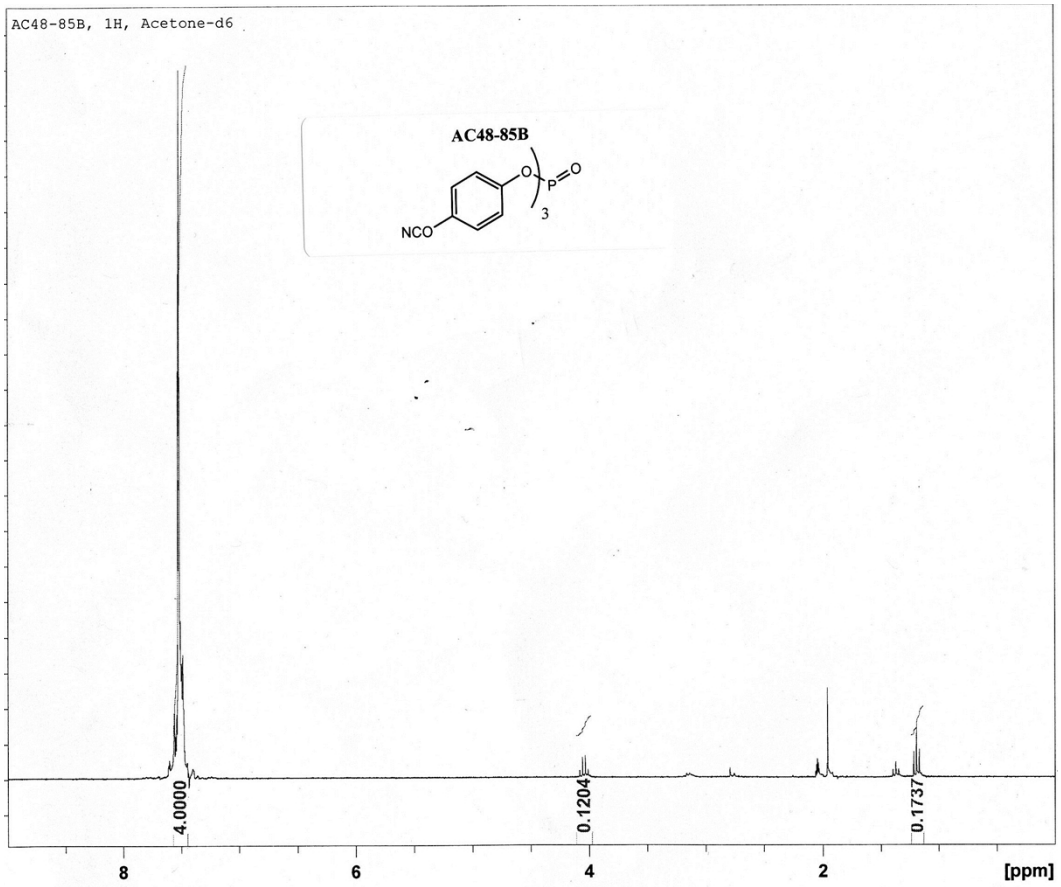

Figure S5. ^{1}H NMR spectrum of PhosCy3 (peaks at 4.05, 1.97 and 1.20 are from ethyl acetate)

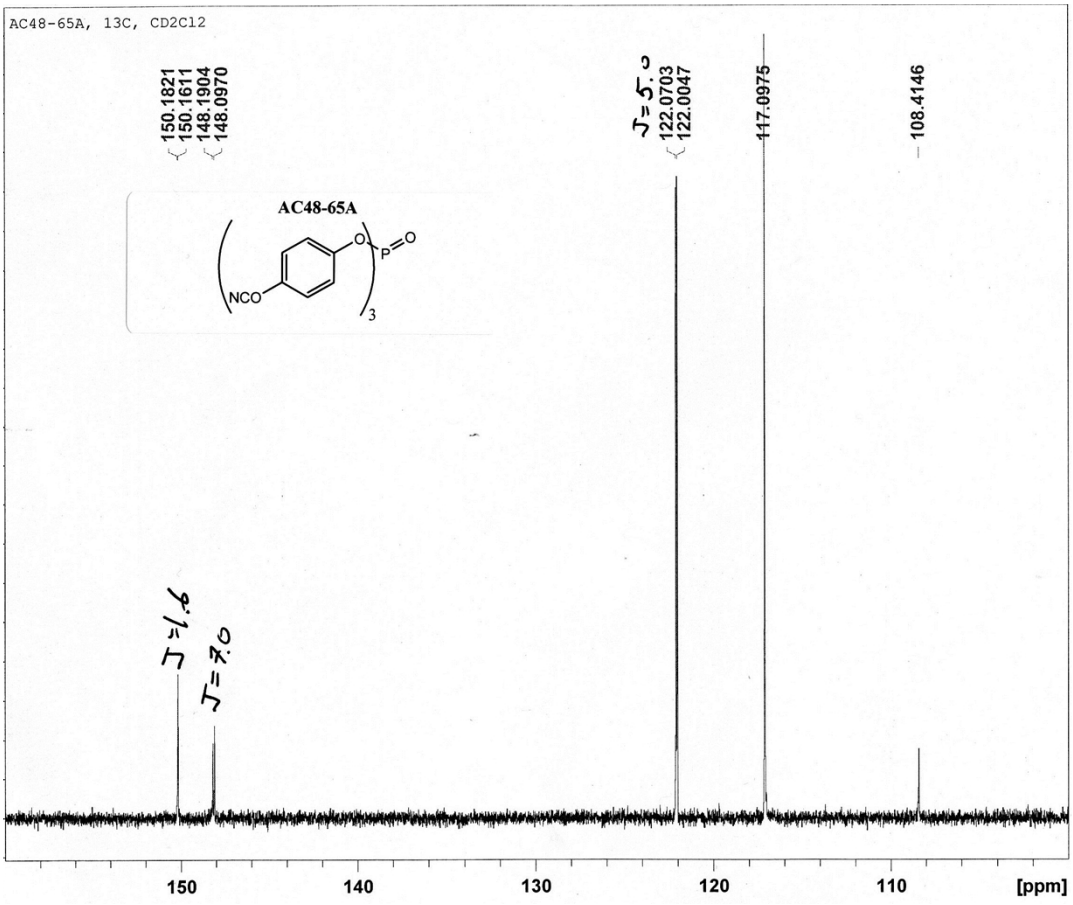

Figure S6. ^{13}C NMR spectrum of PhosCy3

Table S1. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for PhosCy3

	x/a	y/b	z/c	U(eq)
P1	0.3333	0.6667	0.99518(14)	0.0413(2)
O2	0.39714(15)	0.60188(15)	0.0887(2)	0.0512(4)
O1	0.3333	0.6667	0.8032(4)	0.0495(7)
C1	0.5084(2)	0.6112(2)	0.0348(3)	0.0416(5)
O3	0.8264(2)	0.6105(2)	0.9122(4)	0.0787(6)
C3	0.6256(3)	0.5121(3)	0.0217(4)	0.0551(6)
C5	0.7118(2)	0.7198(2)	0.9217(4)	0.0502(6)
C4	0.7192(2)	0.6167(3)	0.9521(3)	0.0511(6)
C2	0.5174(2)	0.5083(2)	0.0640(3)	0.0504(6)
C6	0.6034(2)	0.7171(2)	0.9651(3)	0.0477(6)
N1	0.9990(3)	0.7710(4)	0.7602(6)	0.1043(12)
C7	0.9167(3)	0.6999(4)	0.8321(5)	0.0743(9)

Table S2. Bond lengths (Å) for PhosCy3

P1-O1	1.451(3)	C1-C6	1.376(3)
P1-O2	1.5710(17)	O3-C7	1.284(5)
O2-C1	1.407(3)	C3-C4	1.361(4)
C1-C2	1.375(3)	C5-C4	1.367(4)
O3-C4	1.424(3)	N1-C7	1.116(5)
C3-C2	1.378(4)		
C5-C6	1.389(4)		

Table S3. Bond angles (°) for PhosCy3

O1-P1-O2	116.73(8)	C6-C1-C2	122.3(2)
O2-P1-O2	101.34(9)	C2-C1-O2	115.1(2)
O2-P1-O2	101.34(9)	C4-C3-C2	119.1(2)
C1-O2-P1	125.01(15)	C5-C4-C3	123.2(2)
C6-C1-O2	122.6(2)	C3-C4-O3	114.5(2)
C7-O3-C4	119.9(3)	C1-C6-C5	118.9(2)
C4-C5-C6	118.0(2)		
C5-C4-O3	122.3(3)		
C3-C2-C1	118.5(2)		
N1-C7-O3	173.9(4)		

Table S4. Anisotropic atomic displacement parameters (Å^2) for PhosCy3.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	0.0375(3)	0.0375(3)	0.0488(5)	0	0	0.01876(14)
O2	0.0466(9)	0.0493(9)	0.0603(10)	0.0103(8)	0.0062(7)	0.0258(8)
O1	0.0483(10)	0.0483(10)	0.0518(16)	0	0	0.0242(5)
C1	0.0409(11)	0.0416(11)	0.0452(12)	-0.0020(9)	-0.0048(9)	0.0227(10)
O3	0.0600(13)	0.0872(15)	0.1086(17)	0.0003(13)	0.0019(11)	0.0516(12)
C3	0.0647(17)	0.0488(14)	0.0653(16)	-0.0009(12)	-0.0080(13)	0.0386(13)
C5	0.0422(12)	0.0454(13)	0.0599(14)	-0.0003(11)	-0.0014(11)	0.0194(11)
C4	0.0476(13)	0.0605(16)	0.0548(14)	-0.0100(11)	-0.0109(10)	0.0341(13)
C2	0.0574(15)	0.0385(12)	0.0548(13)	0.0029(11)	-0.0033(12)	0.0235(12)
C6	0.0479(14)	0.0391(12)	0.0599(15)	0.0017(10)	-0.0024(11)	0.0246(11)
N1	0.0568(17)	0.133(3)	0.114(2)	-0.014(2)	0.0054(17)	0.040(2)
C7	0.0500(16)	0.098(3)	0.082(2)	-0.0188(18)	-0.0098(16)	0.0425(18)

The anisotropic atomic displacement factor exponent takes the form: -2π2[h2 a*2 U11 + ... + 2 h k a* b* U12]

Table S5. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å²) for PhosCy3.

	x/a	y/b	z/c	U(eq)
H4	0.593(2)	0.789(3)	0.949(3)	0.048(7)
H3	0.781(3)	0.792(3)	0.876(4)	0.060(8)
H2	0.631(3)	0.446(3)	1.039(4)	0.070(9)
H1	0.451(3)	0.438(3)	1.118(4)	0.052(7)

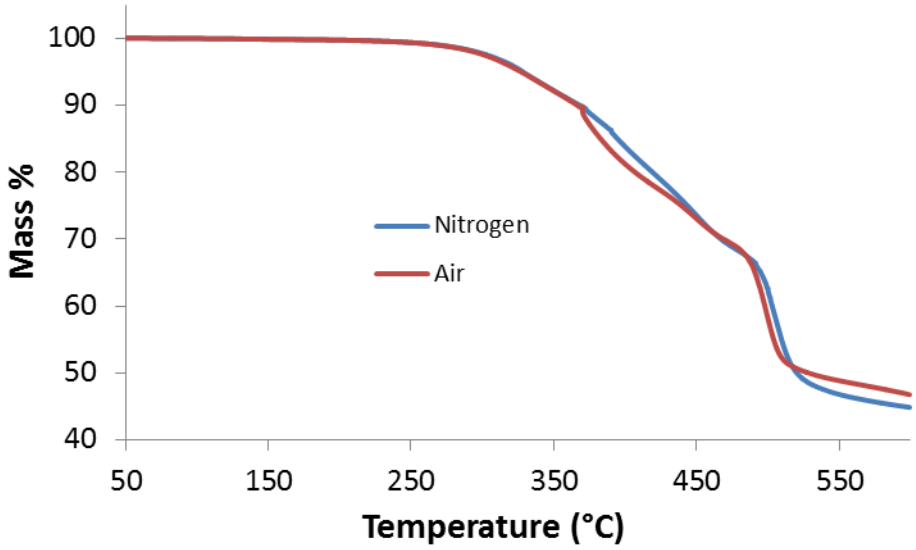

Figure S7. TGA data for PhosCy

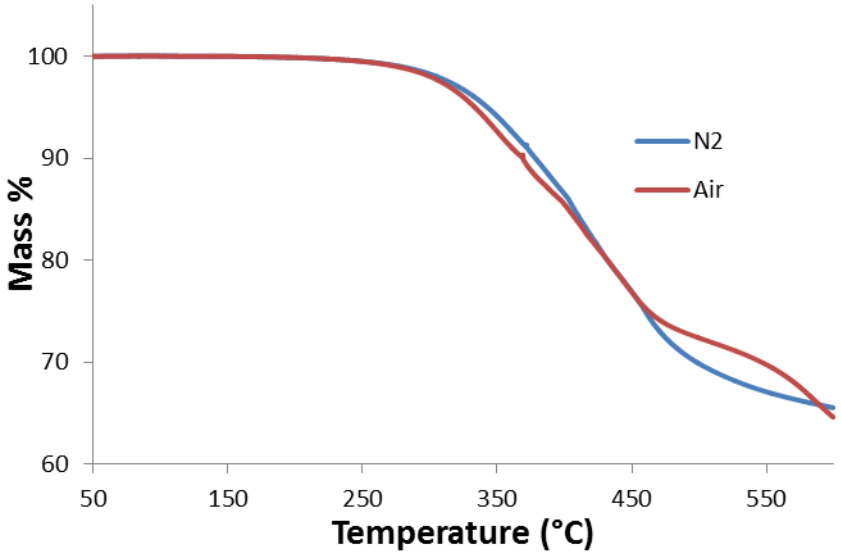

Figure S8. TGA data for MPhosCy

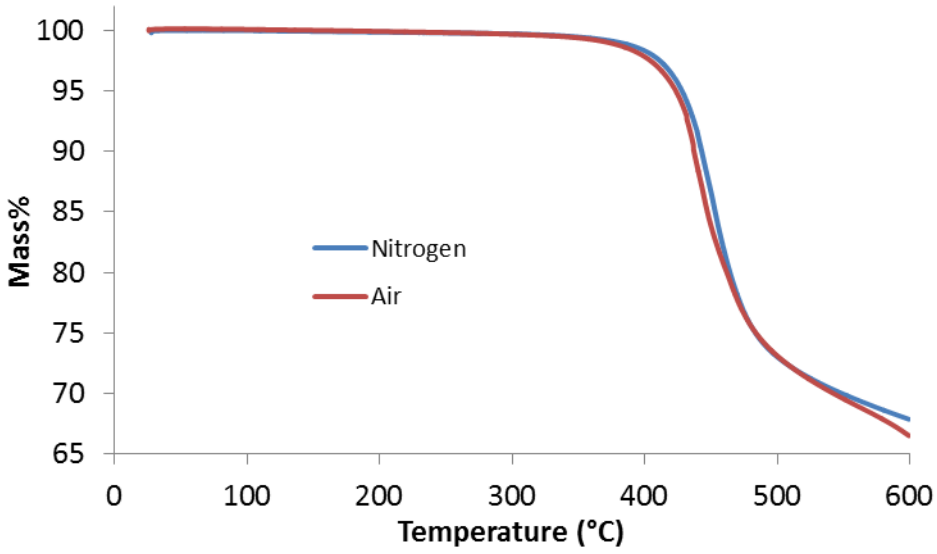

Figure S9. TGA data for PhosCy3

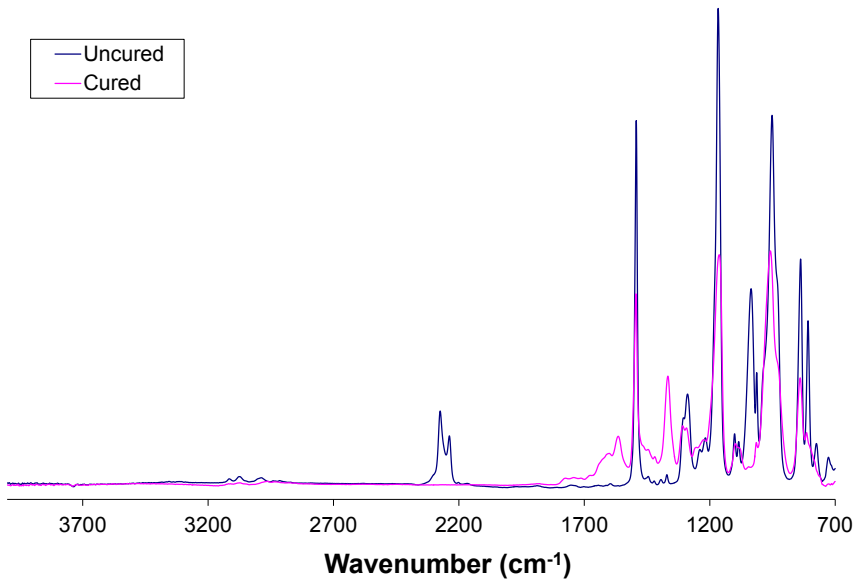

Figure S10. Comparative FTIR data for PhosCy

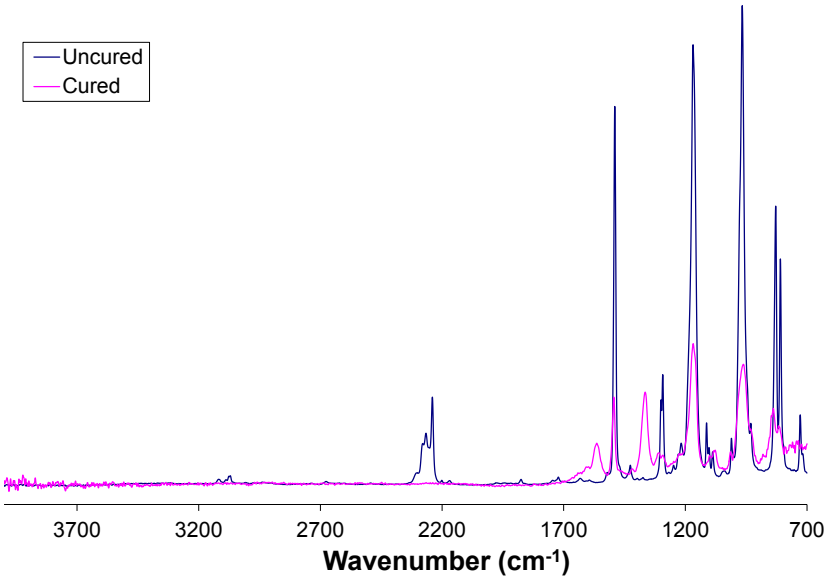

Figure S11. Comparative FTIR data for MPhosCy

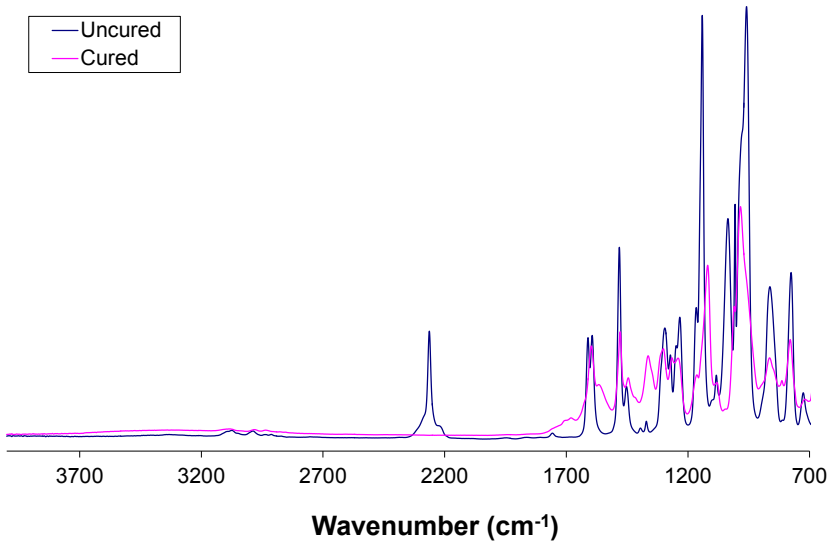

Figure S12. Comparative FTIR data for PhosCy3

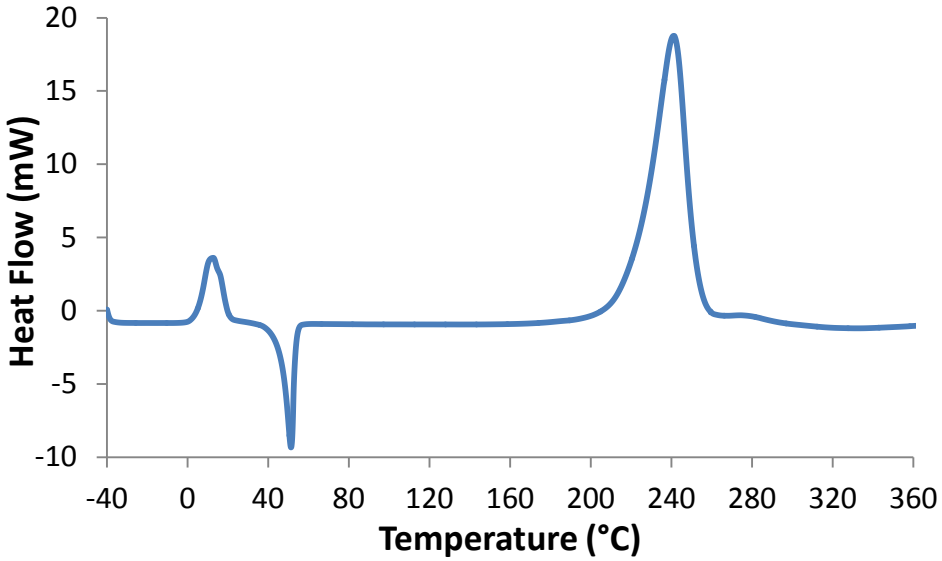

Figure S13. DSC data for PhosCy

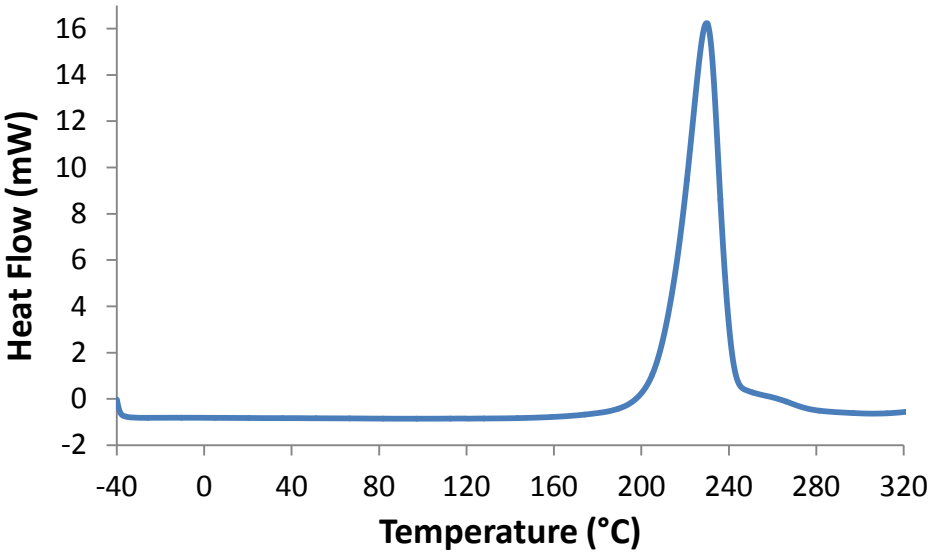

Figure S14. DSC data for MPhosCy

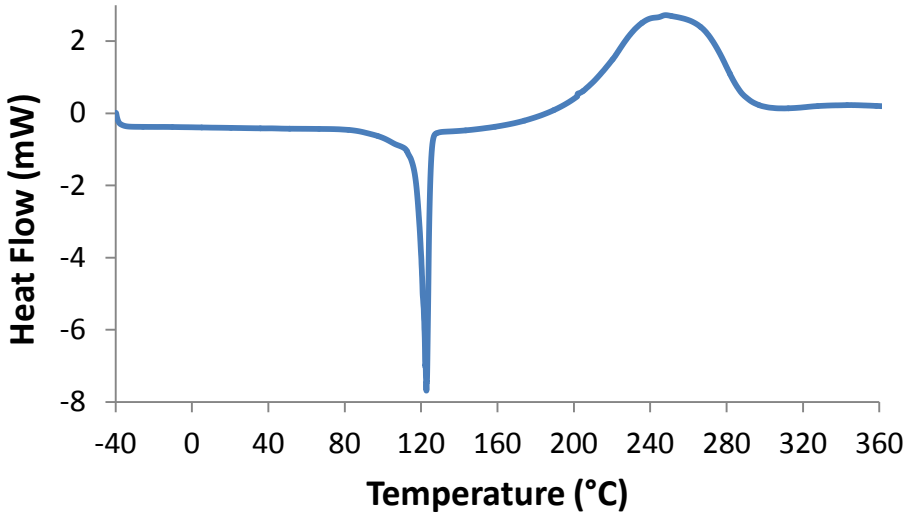

Figure S15. DSC data for PhosCy3

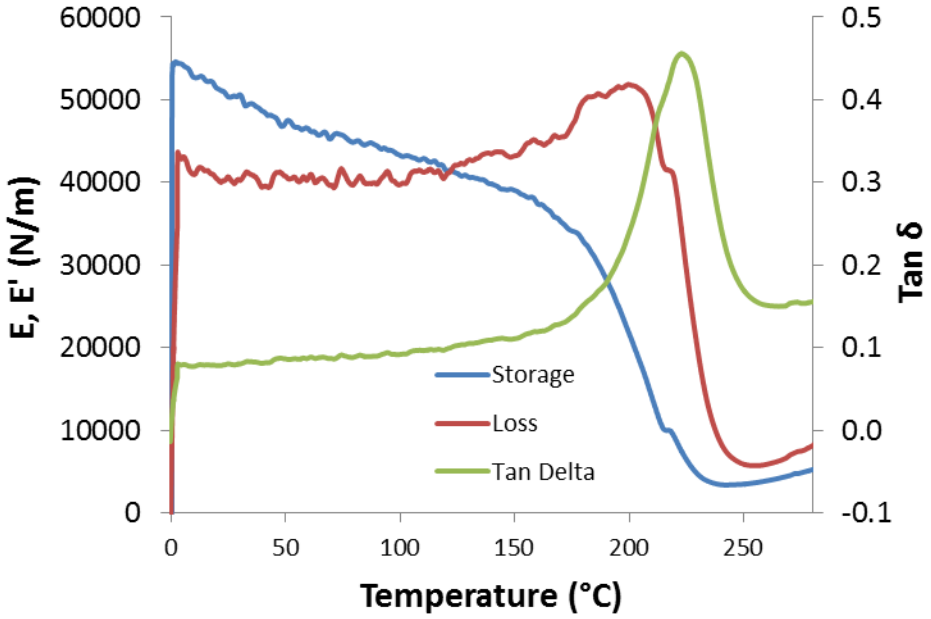

Figure S16. TMA data for PhosCy (loss peak is multiplied by a factor of ten for comparison purposes)

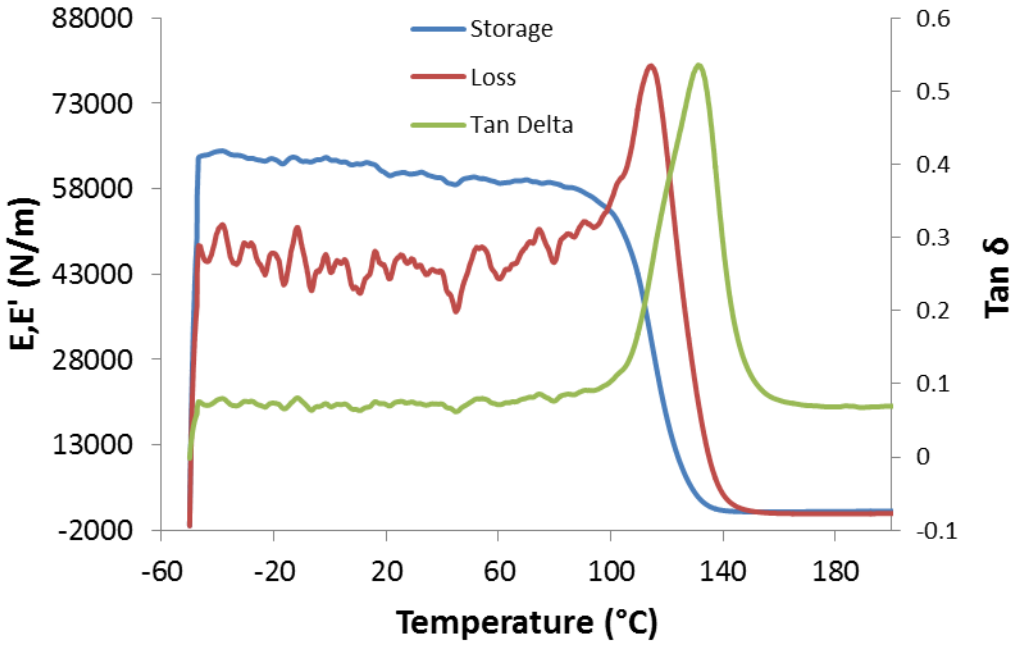

Figure S17. TMA data for MPhosCy (loss peak is multiplied by a factor of ten for comparison purposes)

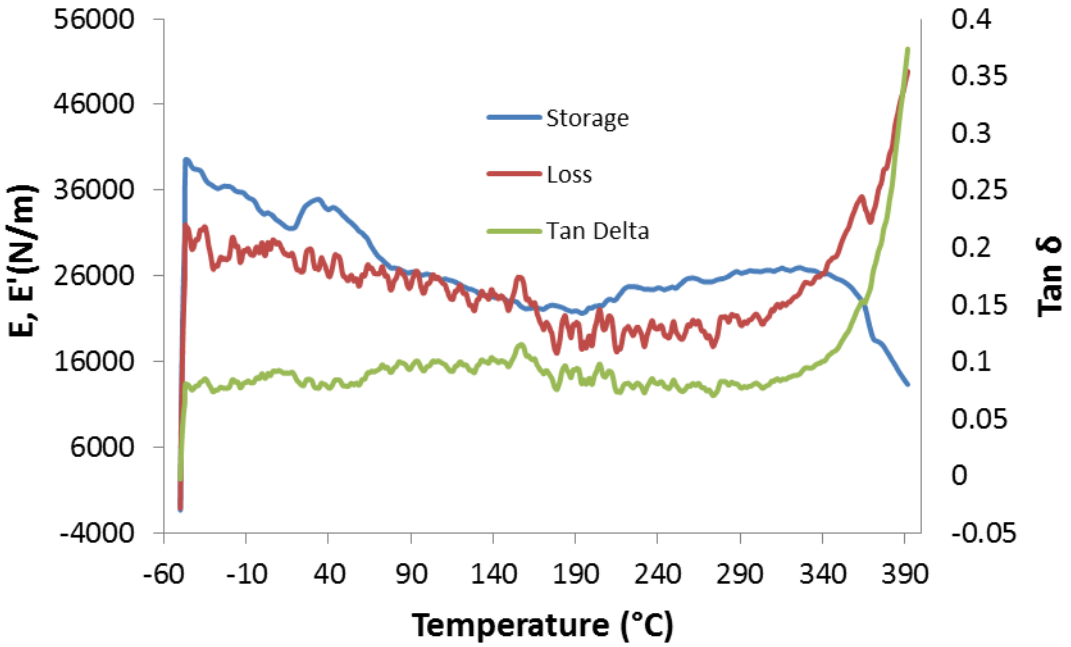

Figure S18. TMA data for PhosCy3 (loss peak is multiplied by a factor of ten for comparison purposes)