Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for

Synthesis and thermally induced structural transformation of phthalimide and nitrile-functionalized benzoxazine: toward smart *ortho*-benzoxazine chemistry for low flammability thermosets

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Synthesis of 2-(2-Hydroxyphenyl)-isoindoline-1,3-dione (*o*-PP)

Into a 250 mL round flask were placed phthalic anhydride (7.41 g, 005 mol), *o*-aminophenol (5.41 g, 0.05 mol), and 60 ml of acetic acid. The mixture was stirred and refluxed for 6 h. After cooling to room temperature, the precipitate was filtered and washed with 200 mL of methanol. Removal of solvent by evaporation afforded an orange crystal (yield ca. 90%). ^{1}H NMR (DMSO), ppm: δ = 6.82-7.93 (8H, Ar), 9.76 (OH). IR spectra (KBr, cm^{-1}) = 3383 (O-H stretching), 1787, 1700 (Imide Ⅰ), 1390 (imide Ⅱ,C-N stretching), 722 (C=O bending).

Synthesis of 2-(3-Phenyl-3,4-dihydro-2*H*-benzo[*e*][1,3]oxazin-8-yl)-isoindoline-1,3-dione (*o*PP-a)

Into a 100 mL round flask were added 30 mL of xylenes, aniline (1.40 g, 0.15mol), *o*-PP (3.59 g, 0.015mol), and paraformaldehyde (0.91g, 0.03 mol). The mixture was stirred at 120 ^{o}C for 6 h. The mixture was cooled to room temperature and precipitated into 100 mL of methanol. Removal of solvent by filtering afforded a yellow powder. (yield ca. 95%, m.p. 209 ^{o}C). ^{1}H NMR (DMSO), ppm: δ = 4.72 (s, Ar-CH_2-N, oxazine), 5.42 (s, O-CH_2-N, oxazine), 6.85-7.96 (12H, Ar). IR spectra (KBr), cm^{-1}: 1774, 1719 (imide I), 1497 (stretching of trisubstituted benzene ring), 1385 (imide II), 1231 (C-O-C asymmetric stretching), 1179 (C-N-C asymmetric stretching), 924 (out-of-plane C-H).

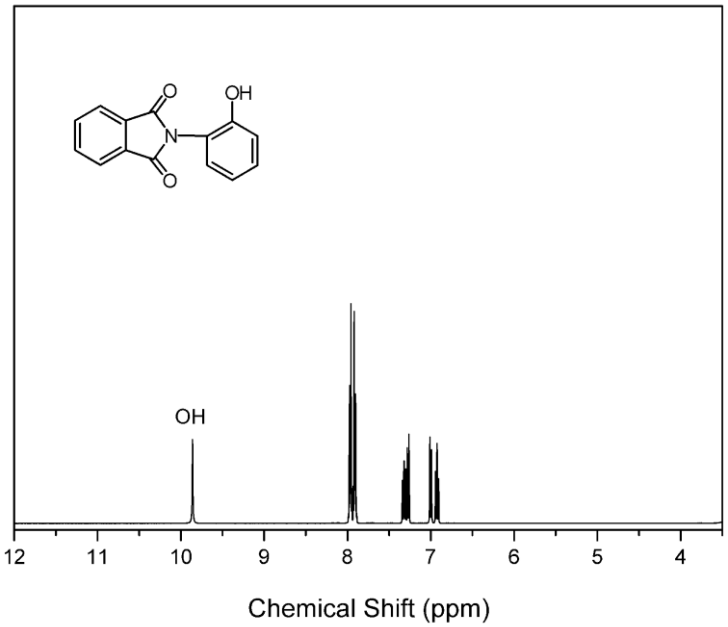

Figure S1. ^{1}H NMR spectrum of *o*PP.

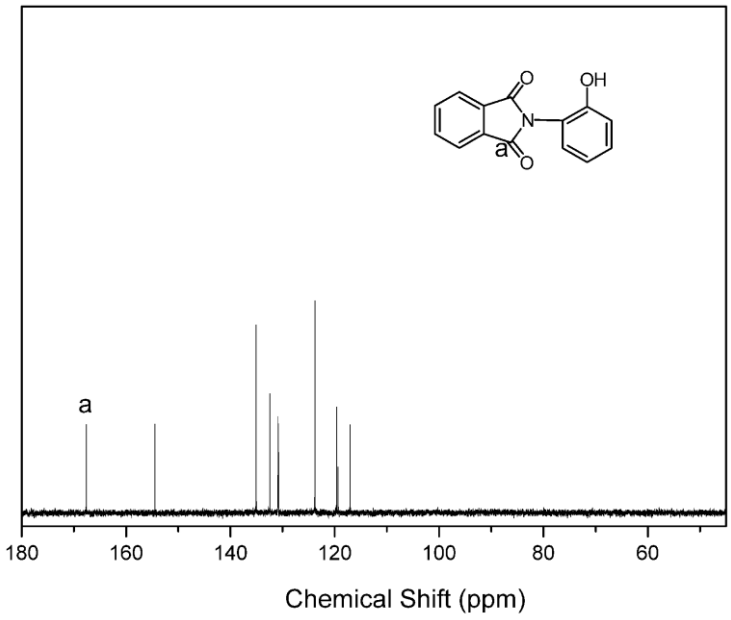

Figure S2. ^{13}C NMR spectrum of *o*PP.

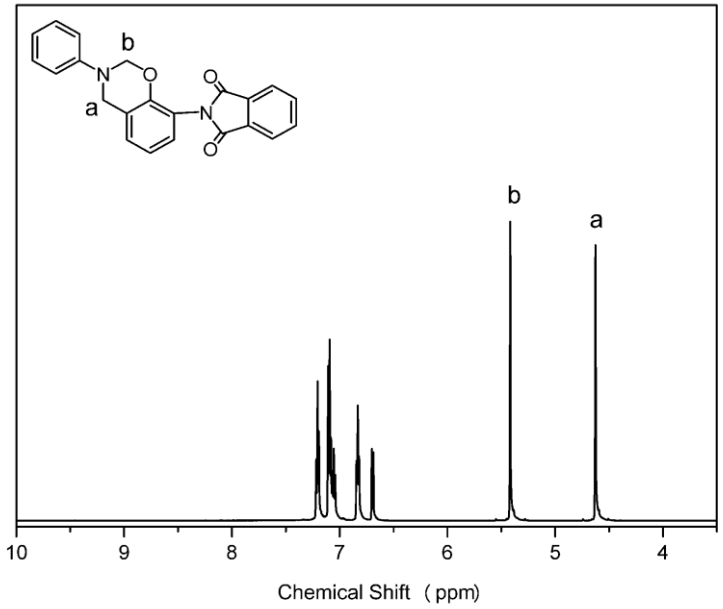

Figure S3. ^{1}H NMR spectrum of *o*PP-a.

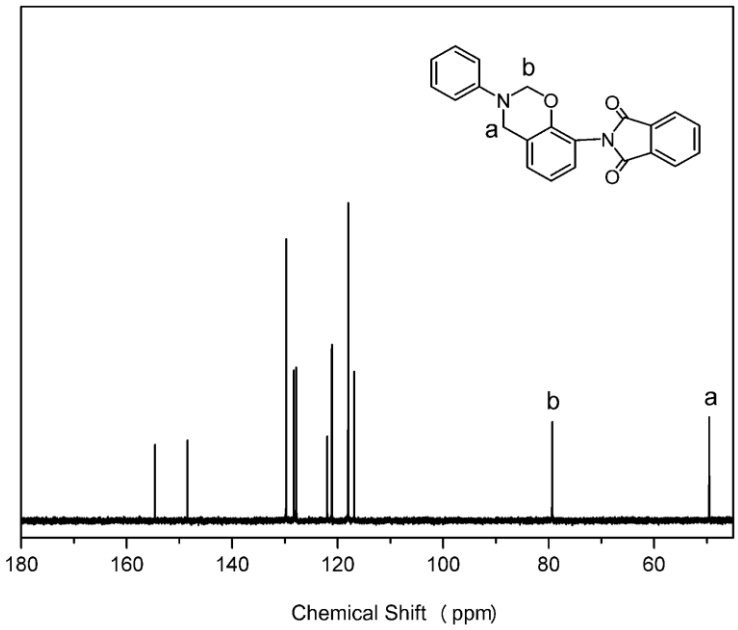

Figure S4. ^{13}C NMR spectrum of *o*PP-a.

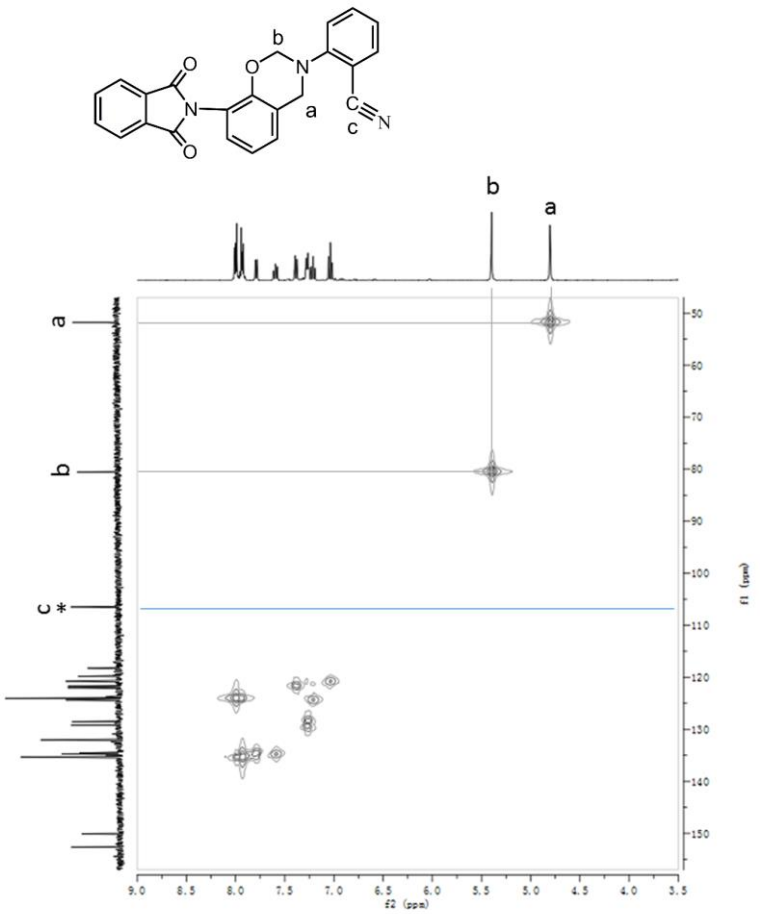

Figure S5. ^{1}H-^{13}C HMQC spectrum of *o*PP-an.

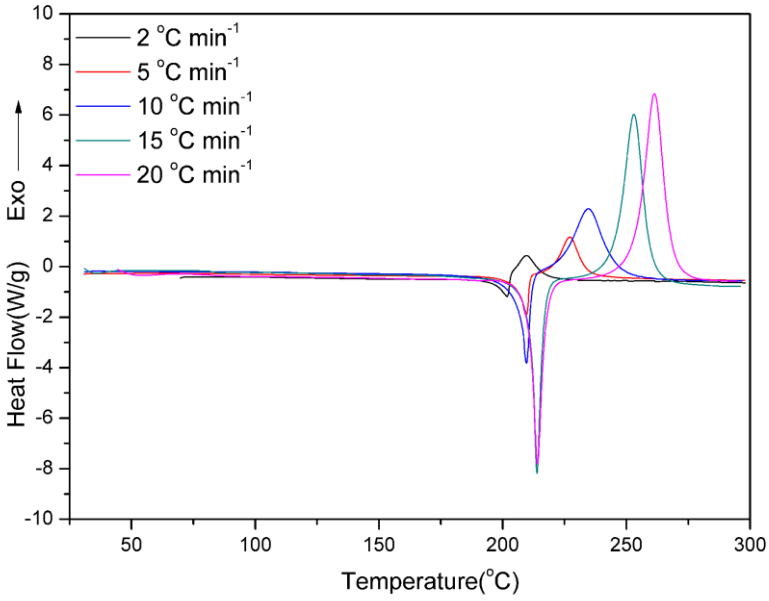

Figure S6. DSC curves of *o*PP-a at different heating rates.

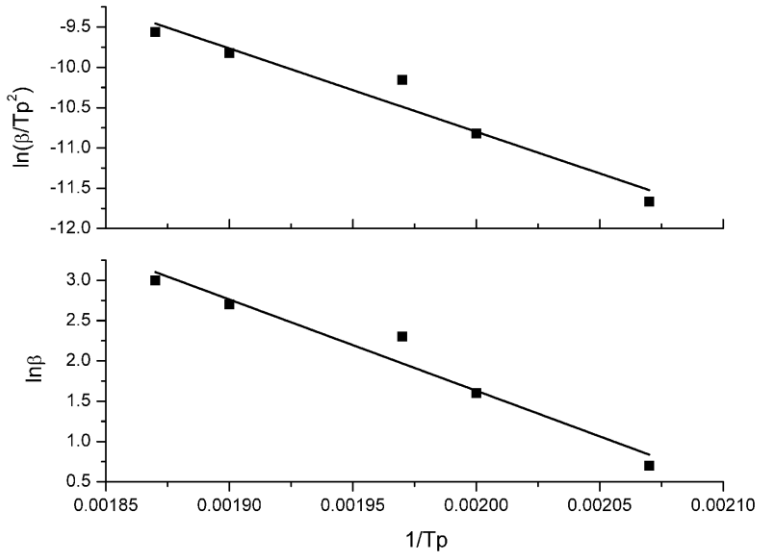

Figure S7. Representations of Kissinger and Ozawa methods for the calculation of activation energy for *o*PP-a.

Table S1. The Activation Energy of *o*PP-a obtained by Kissinger and Ozawa Methods.

Sample	Kissinger	Ozawa
	Ea (kJ/mol)	*Ea* (kJ/mol)
*o*PP-a	86.0	89.5