

Supplementary Material

A novel benzoxazine/cyanate ester blend with sea-island phase structures

Xiaodan Li,^{1,2} Xiaoyong Luo² and Yi Gu² □

¹Key Laboratory of Catalysis Science and Technology of Chongqing Education Commission, College of Environment and Biological Engineering, Chongqing Technology and Business University, Chongqing, 400067, P.R. China

²State Key Laboratory of Polymer Materials Engineering, College of Polymer Sciences and Engineering, Sichuan University, Sichuan, Chengdu 610065, P. R. China

Characterization of P-BOZ

Melting point: 128 °C; IR (KBr): 941 cm⁻¹ (s, oxazine ring).

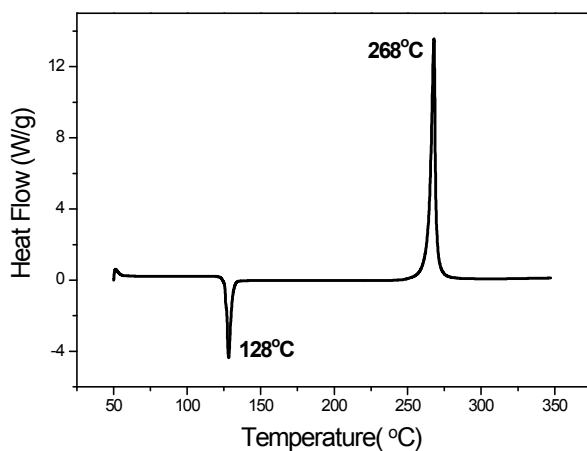


Fig. 1. DSC curve of P-BOZ.

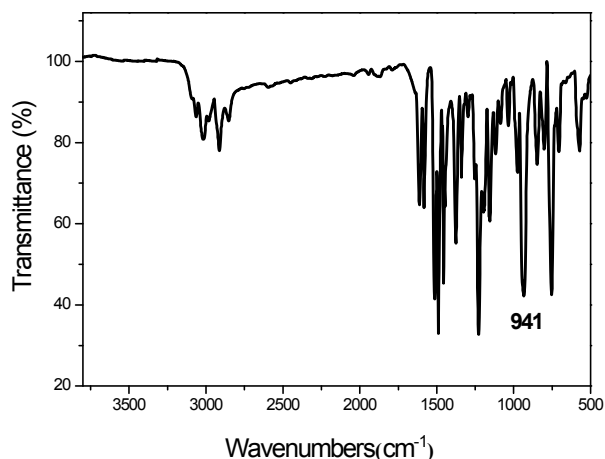


Fig. 2. FT-IR spectrum of P-BOZ.

Characterization of C-BOZ

Melting point: 95 °C; IR (KBr): 2921 cm^{-1} , 2851 cm^{-1} (vs, $\nu_s(-\text{CH}_2)$), 960 cm^{-1} (s, oxazine ring).

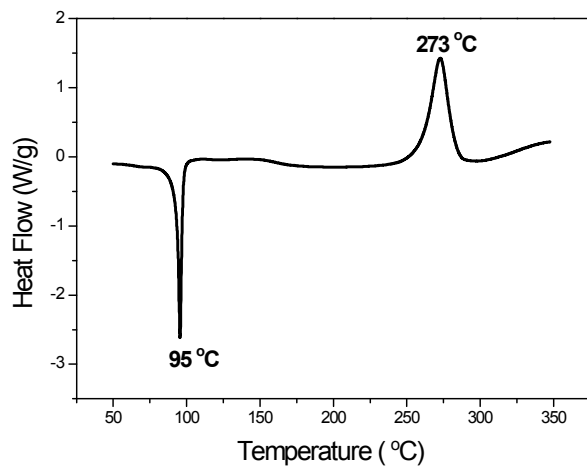


Fig. 3. DSC curve of C-BOZ.

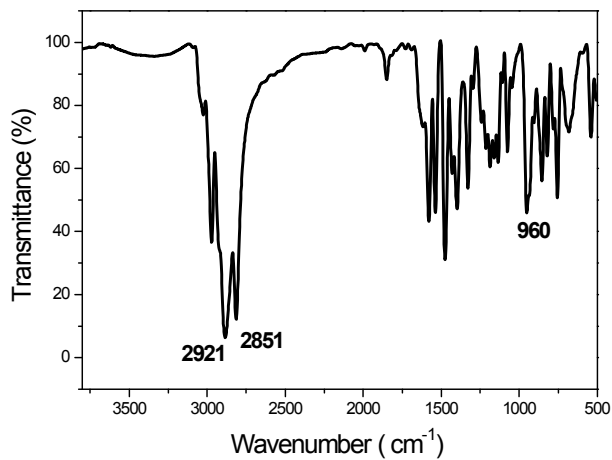


Fig. 4. FT-IR spectrum of C-BOZ.

Characterization of BADCy

Melting point: 83 °C; IR (KBr): 2227 cm^{-1} , 2275 cm^{-1} (vs, $\nu_s(-\text{OCN})$).

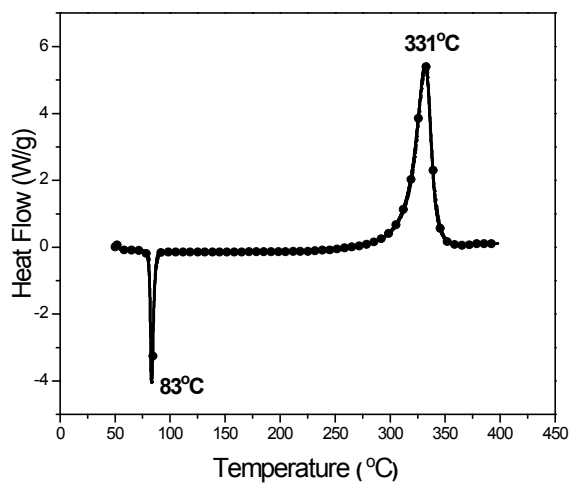


Fig. 5. DSC curve of BADCy.

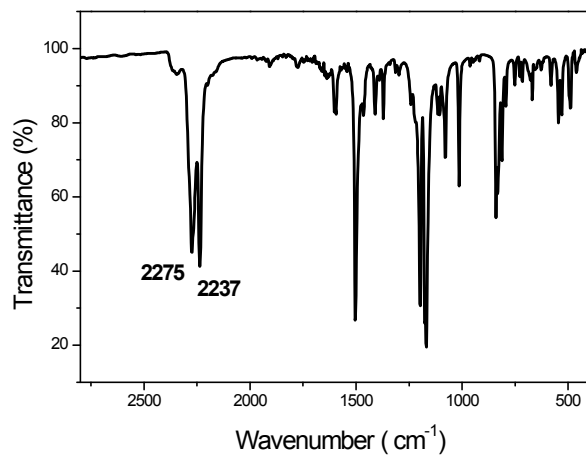


Fig. 6. FT-IR spectrum of BADCy.

Calculation of Flory-Huggins interaction parameters

Mole gravitational constants of all groups are shown in Table 1. The Flory-Huggins interaction parameters, χ , were estimated as follows.

Table 1. Molar gravitational constants of different groups.

	-CH ₃	-CH=	-C≡N	-O-	-CH ₂ -	-C-
Molar gravitational constant (J/M ³) ^{0.5}	301.4	434.87	725.5	235.3	269.1	65.54

$$\rho_{\text{BADCy}}=1.22\text{g/cm}^3 \quad \rho_{\text{P-BOZ}}=1.21 \text{ g/cm}^3 \quad \rho_{\text{C-BOZ}}=0.95 \text{ g/cm}^3$$

$$\delta_{\text{BADCy}} = \frac{\sum F_i}{V_R} = \frac{\rho}{M} \sum F_i = \frac{1.22}{278} \times 5309.94 = 23.30(\text{J/cm}^3)^{0.5}$$

$$\delta_{\text{C-BOZ}} = \frac{\sum F_i}{V_R} = \frac{\rho}{M} \sum F_i = \frac{0.95}{852.5} \times 15241.72 = 16.98(\text{J/cm}^3)^{0.5}$$

$$\delta_{\text{P-BOZ}} = \frac{\sum F_i}{V_R} = \frac{\rho}{M} \sum F_i = \frac{1.21}{434.5} \times 7657.7 = 21.33(\text{J/cm}^3)^{0.5}$$

P-BOZ/BADCy (5/5 for example):

$$V_{\text{ref}} = M_a \phi_a / \rho_a + M_b \phi_b / \rho_b = \frac{278}{1.22} \times 0.5 + \frac{434.5}{1.21} \times 0.5 = 293.48 \text{ cm}^3$$

$$\chi_{\text{P-BOZ/BADCy}} = \frac{V_{\text{ref}}}{RT} (\delta_{\text{P-BOZ}} - \delta_{\text{BADCy}})^2 = \frac{293.48}{8.314 \times 298} \times (21.33 - 23.30)^2 = 0.46$$

C-BOZ/BADCy (5/5 for example):

$$V_{\text{ref}} = M_a \phi_a / \rho_a + M_b \phi_b / \rho_b = \frac{278}{1.22} \times 0.5 + \frac{852.5}{0.95} \times 0.5 = 562.62 \text{ cm}^3$$

$$\chi_{\text{C-BOZ/BADCy}} = \frac{V_{\text{ref}}}{RT} (\delta_{\text{C-BOZ}} - \delta_{\text{BADCy}})^2 = \frac{562.62}{8.314 \times 298} \times (16.98 - 23.30)^2 = 9.07$$