Supplementary Information (SI) for Inorganic Chemistry Frontiers.

Supporting Information

A Covalent Organic Polymer Containing Dative B←N Bonds: Synthesis, Single Crystal Structure, and Physical Properties

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Materials

All the reagents for the synthesis of **CityU-30** are indicated as follows: 9,10-di(4-pyridyl)anthracene (Zhengzhou Alfa Chemical Co., Ltd., 98%), 1,4-phenylenebisboronic acid (Shanghai Aladdin Biochemical Technology co., ltd., 98%), 1,2-dihydroxybenzene (Shanghai Aladdin Biochemical Technology co., ltd., 99%). These reagents were used directly without further purification. All solvents were purchased from Anaqua (Hong Kong) Company Limited and used as received without further purification.

Characterization

The single crystal with suitable size was selected for structural characterization (CCDC number: 2363533). The data were collected on Rigaku XtaLAB PRO II Industrial X-ray diffractometer at 300K. Scanning electron microscope (SEM) was conducted on Thermo Fisher Quattro S Environmental SEM. X-ray photoelectron spectroscopy (XPS) analysis was conducted on a Thermo Fisher ESCALAB XI+ X-ray Photoelectron Spectrometer. Powder X-ray diffraction (PXRD) data were collected on Rigaku D2 PHASER XE-T X-ray Diffractometer System with Cu Kα target (λ=1.54056 Å). Fourier-transform infrared spectroscopy (FTIR) spectra were obtained on PerkinElmer Spectrum II. The thermal gravimetric analysis (TGA) of **CityU-30** was carried out on PerkinElmer Simultaneous. The UV-vis absorption data were measured by Hitachi UH4150 UV-VIS-NIR Spectrophotometer. Fluorescent spectroscopy was performed on Horiba FluoroMax-4. The absolute fluorescence quantum yield (PLQY) were measured using Edinburgh Instruments FLS1000 Photoluminescence Spectrometer System. The infrared (IR) images were taken on Fluke Ti480 PRO Infrared Camera.

Table S1. Crystal data and structure refinement of **CityU-30 (**CCDC number: 2363533)

	CityU-30
Empirical formula	$C_{21}H_{14}BNO_2$
Formula weight	323.14
Crystal system	triclinic
Space group	P-1
***a* (Å)**	6.41670(10)
***b* (Å)**	13.1842(4)
***c* (Å)**	13.6585(4)
***α* (°)**	116.729(3)
***β* (°)**	92.641(2)
***γ* (°)**	103.286(2)
***V* (Å^3)**	989.45(5)
Z	2
D_{calc}**(g·cm^{-3})**	1.085
Abs.coeff.(mm^{-1})	0.550
F(000)	336.0
Reflns collected	8380
GOFon F^2	0.973
R_{int}	0.0411
R_1[a]	0.0435
wR_2**(all data)**[b]	0.1425

[a] $R_1=\Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR_2=|\Sigma w\,(|F_o|^2-|F_c|^2)|/\Sigma|w(F_o^2)^2|^{1/2}$

Table S2. Selected bond distances (Å) of **CityU-30**

Atom 1	Atom 2	Length/Å
N1	C12	1.3281 (19)
N1	C10	1.339 (2)
N1	B1	1.690 (2)
O1	C5	1.3667(17)
O1	B1	1.4673(19)
O2	C6	1.3722(17)
O2	B1	1.4572(19)
C1	C2	1.377(3)
C3	C1	1.393(3)
C4	C2	1.392(3)
C5	C6	1.389(2)
C5	C3	1.370(2)
C6	C4	1.374(2)
C8	C9	1.375(2)
C8	B1	1.596(2)
C8	C7	1.376(2)
C9	C7[2]	1.386(2)
C11	C10	1.371(2)
C12	C13	1.381(2)
C15	C14	1.4957(19)
C16	C15	1.405(2)

[1]1-X,2-Y,1-Z; [2]2-X,1-Y,-Z

Table S3. Selected bond angles (°) of **CityU-30**

Atom 1	Atom 2	Atom 3	Angle/°
C5	O1	B1	105.32(11)
C12	N1	B1	123.25(12)
C10	N1	B1	118.21(12)
O1	C5	C6	110.50(12)
O1	C5	C3	127.91(15)
C3	C5	C6	121.58(14)
C9	C8	B1	121.81(14)
C9	C8	C7	115.80(14)
N1	C10	C11	122.17(15)
O1	B1	N1	105.26(11)
O1	B1	C8	117.99(13)
O2	B1	O1	106.89(11)

[1]1-X,2-Y,1-Z; [2]2-X,1-Y, -Z

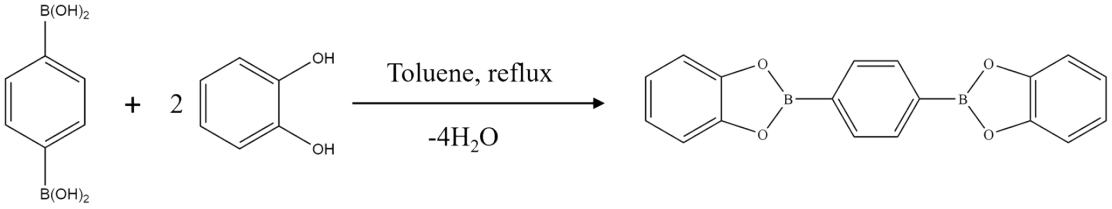

Figure S1. Synthesis of BACT.

Benzene-1,4-diboronic acid (0.5 g) and catechol (0.74 g) were added into 80 mL toluene. The mixture was heated under reflux overnight with a Dean−Stark apparatus device for 48h. After reaction, the solvent was removed by solvent evaporation under reduced pressure. The obtained white needle-like crystals were further dried in vacuum at 120 ℃ for 12 h. Yield: 95%.

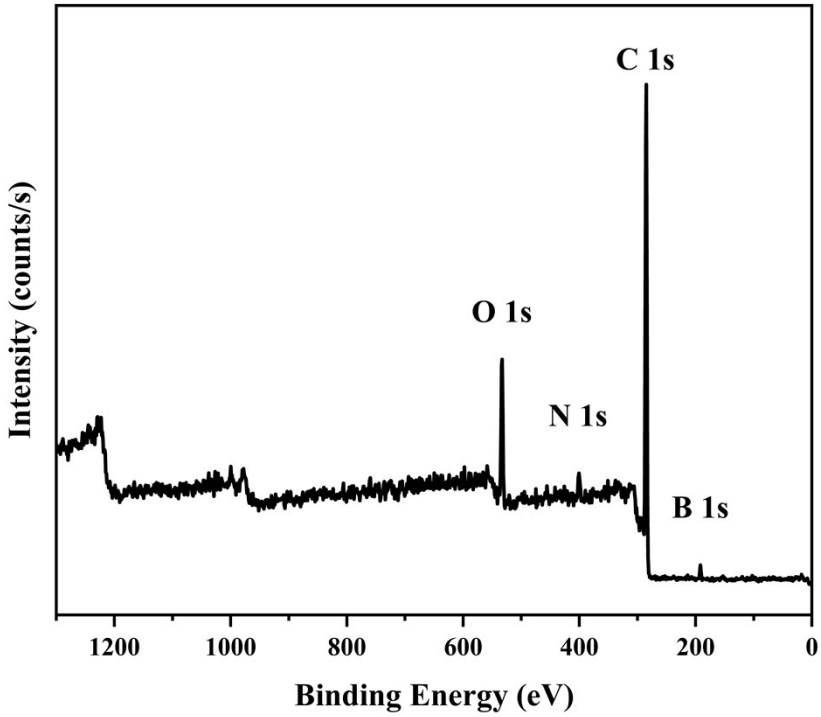

Figure S2. XPS survey of **CityU-30**.

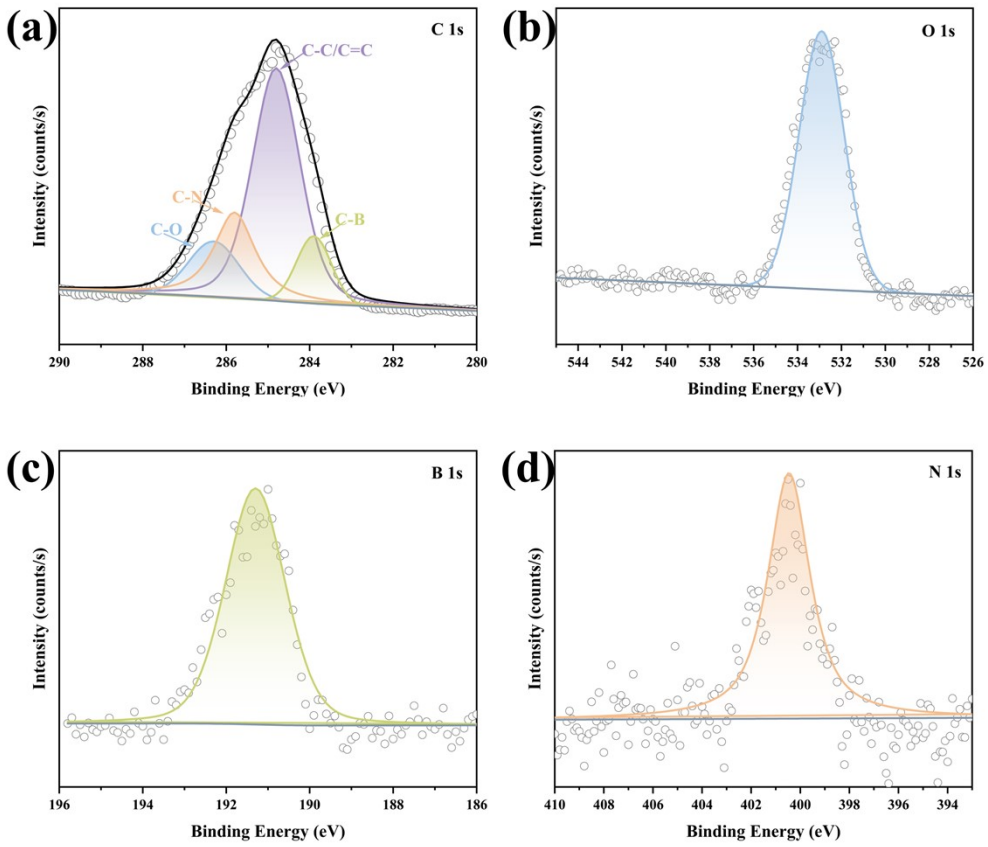

Figure S3. XPS spectra of **CityU-30** on **(a)** C 1s, **(b)** O 1s, **(c)** B 1s, and **(d)** C 1s.

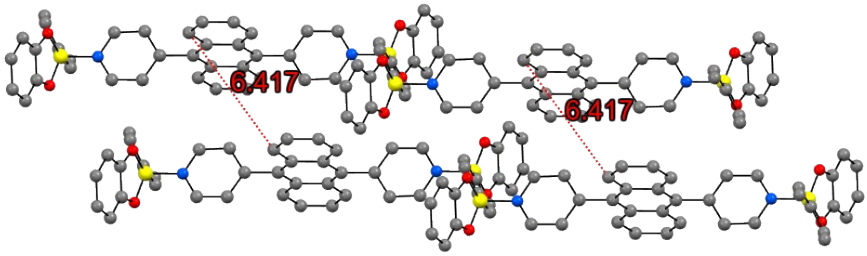

Figure S4. Distance between chains of **CityU-30** (Unit: Å).

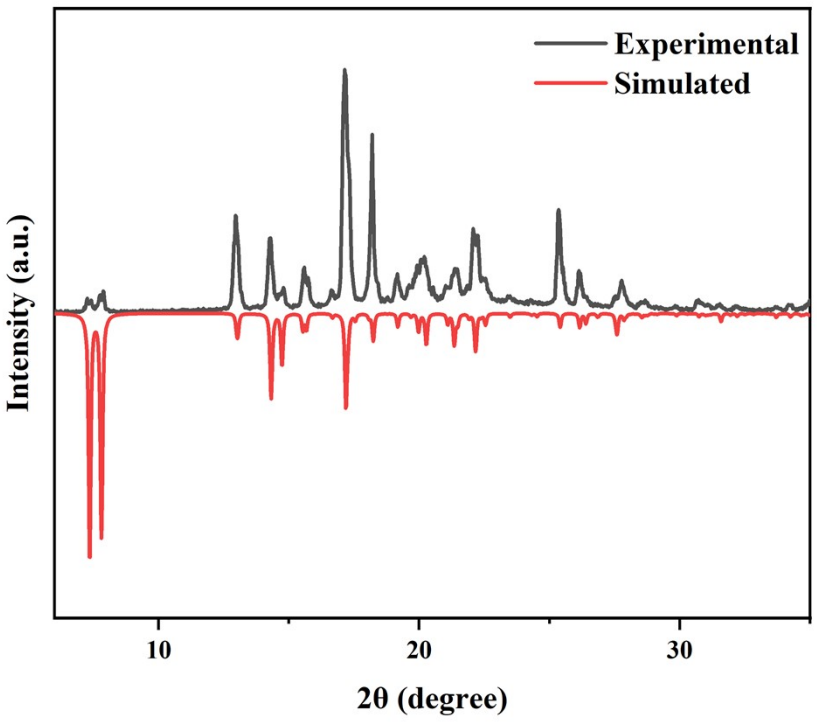

Figure S5. Experimental and simulated PXRD patterns of **CityU-30**.

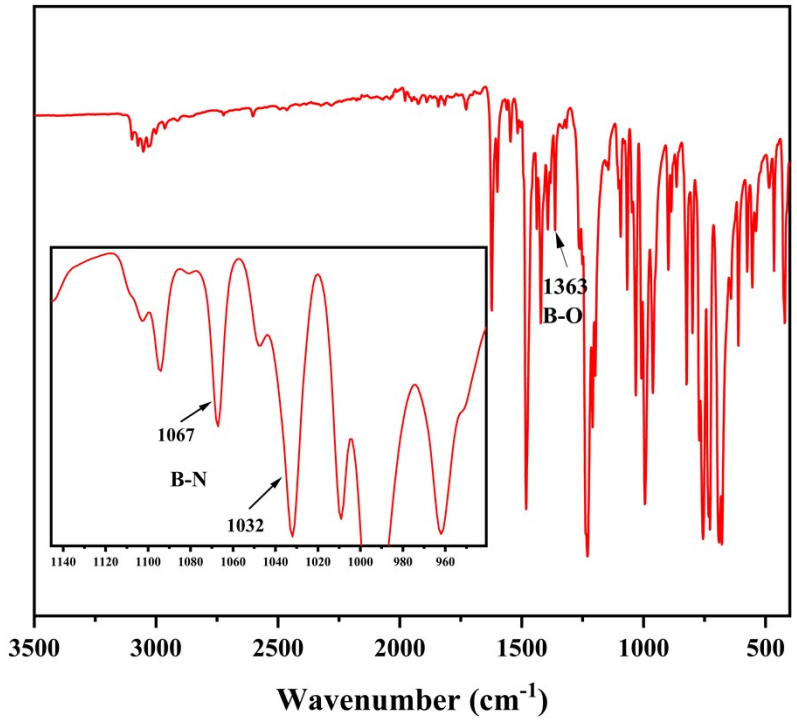

Figure S6. FTIR spectrum of **CityU-30**.

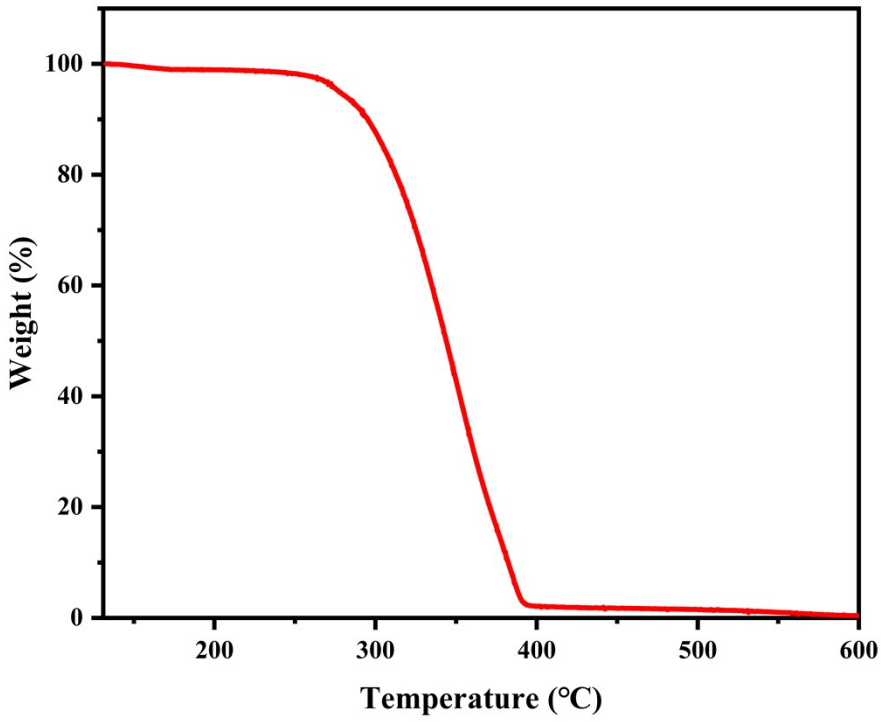

Figure S7. TGA curve of **CityU-30**

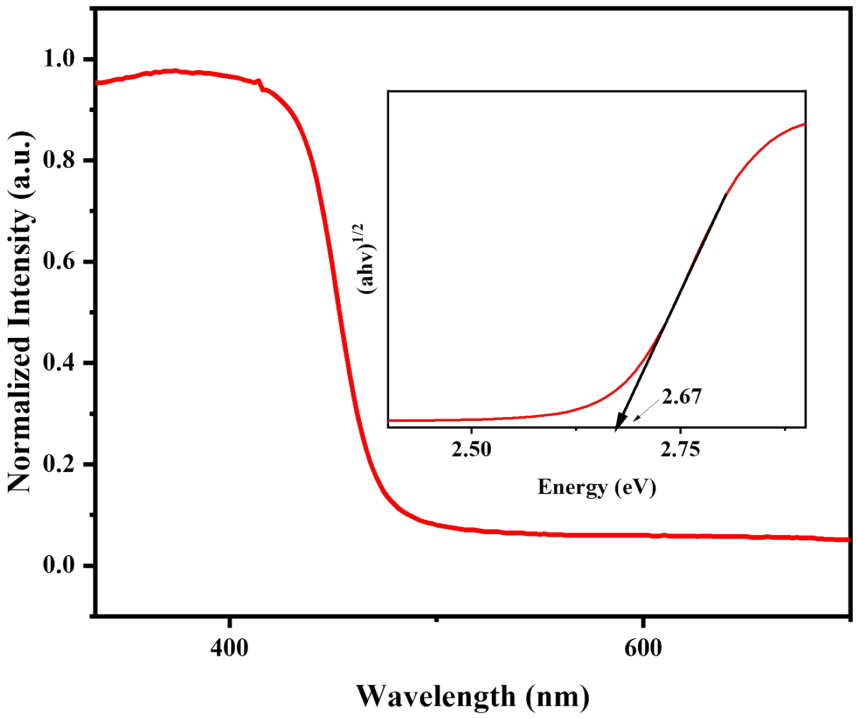

Figure S8. UV-vis spectrum of **CityU-30**. The inset is the curve obtained by Tauc-plot method.

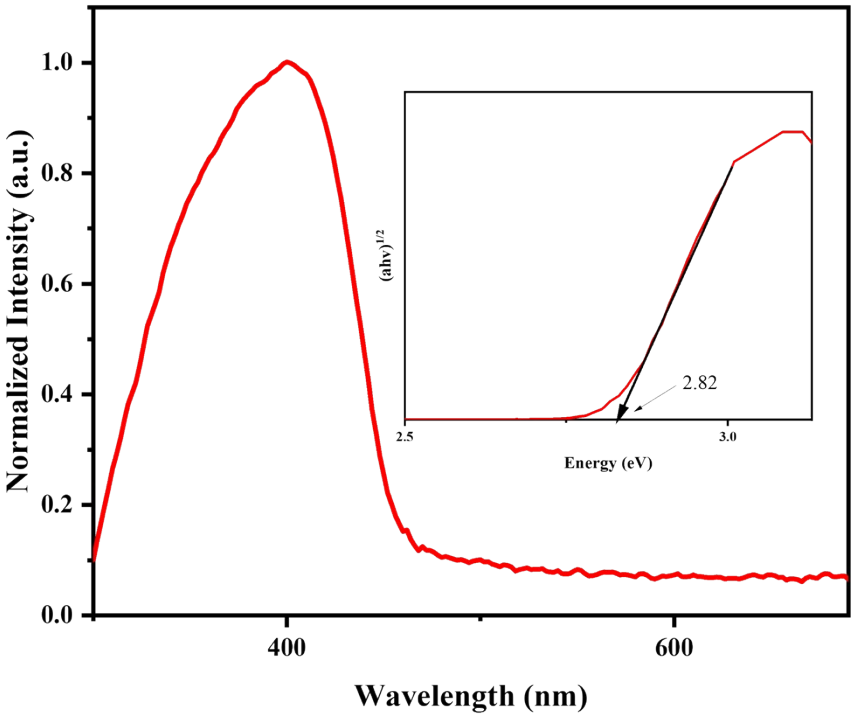

Figure S9. UV-vis spectra of DPA. The inset is the curve obtained by Tauc-plot method.

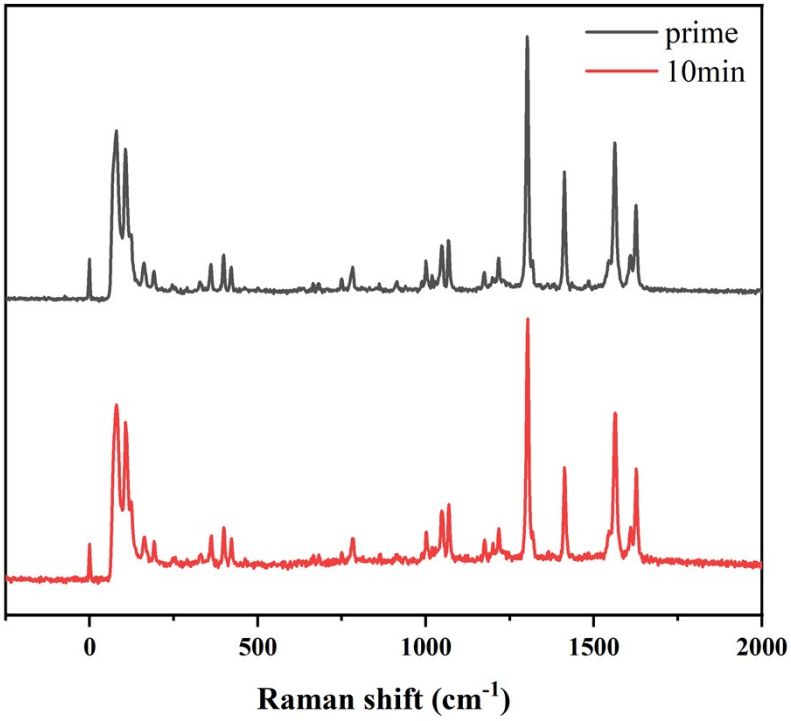

Figure S10. Raman spectra of **CityU-30** before excitation at 396 nm and after 10min of excitation.