Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Information

Explicit analysis of functional-group orientation in amorphous organic semiconductor films by using deuterated materials

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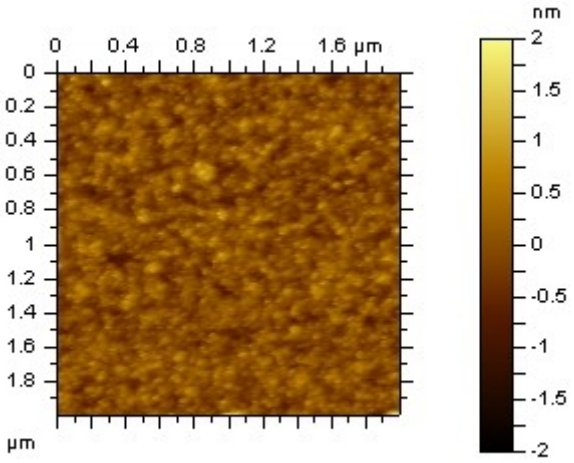

Fig. S1 AFM image of a 100-nm-thick BPBPA-D0 film deposited on a Si(100) substrate. The RMS value of the surface roughness is 0.27 nm.

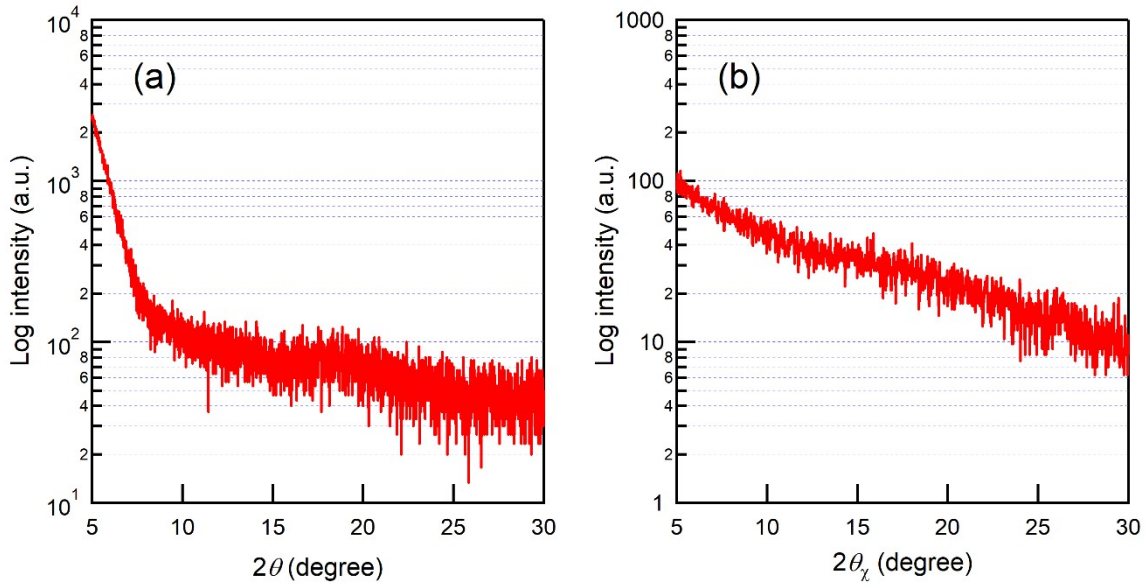

Fig. S2 (a) Out-of-plane and (b) in-plane XRD patterns of a 100-nm-thick BPBPA-D0 film deposited on a Si(100) substrate.

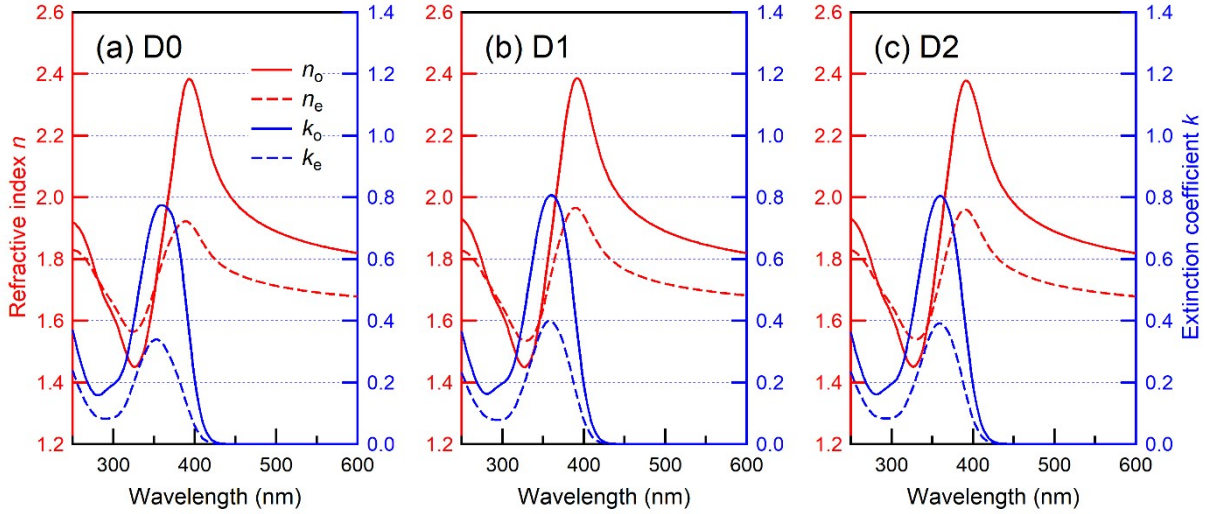

Fig. S3 Anisotropic refractive indices and extinction coefficients of 100-nm-thick as-deposited films of (a) BPBPA-D0, (b) D1, and (c) D2 determined by VASE.

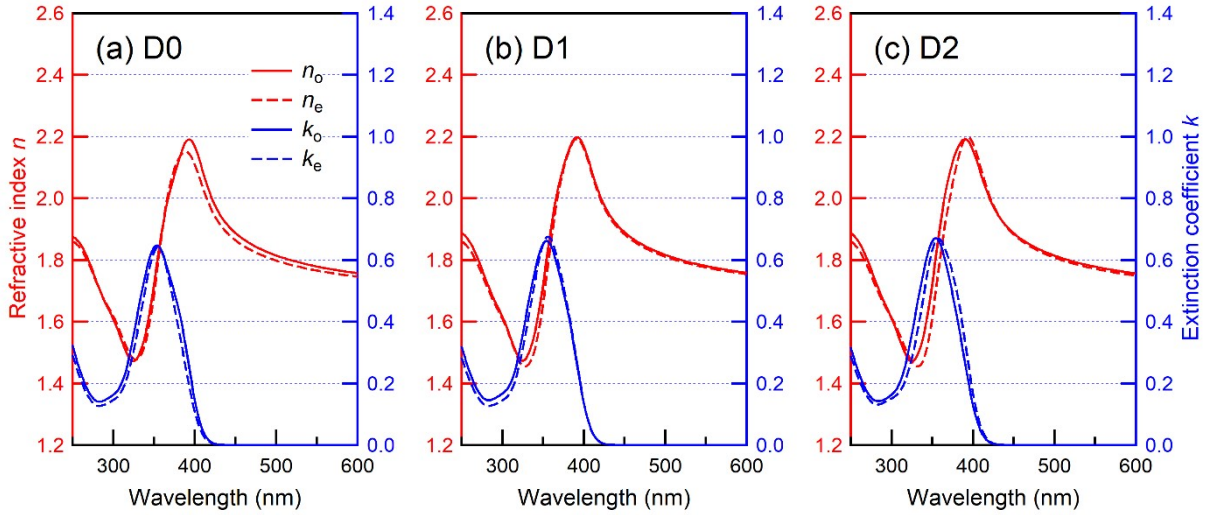

Fig. S4 Anisotropic refractive indices and extinction coefficients of 100-nm-thick annealed films of (a) BPBPA-D0, (b) D1, and (c) D2 determined by VASE.

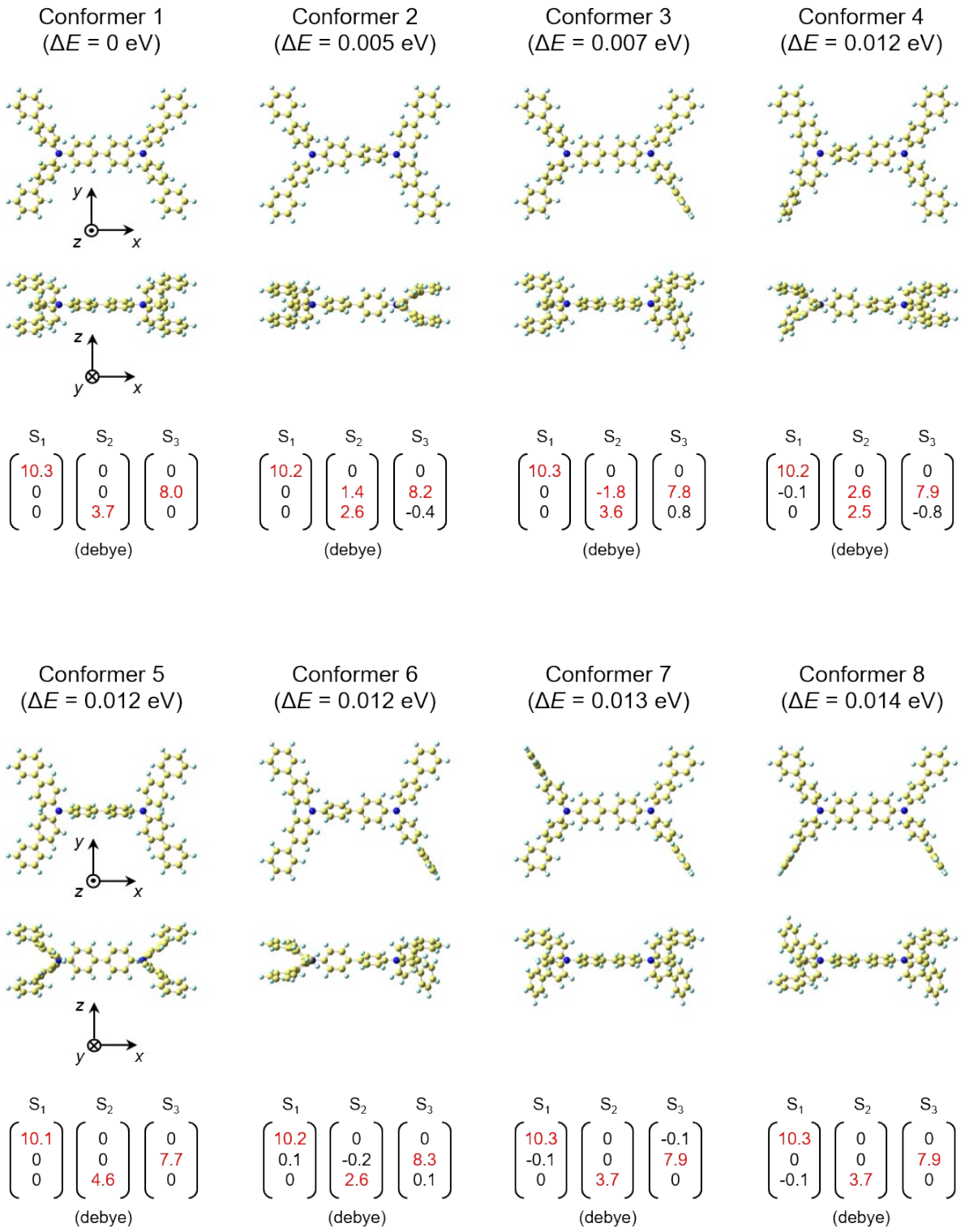

Fig. S5 Steric structures and transition dipole moment vectors for low-energy electronic transitions of the 24 conformers of BPBPA molecules. The differences in the steric energy are also shown as Δ*E*.

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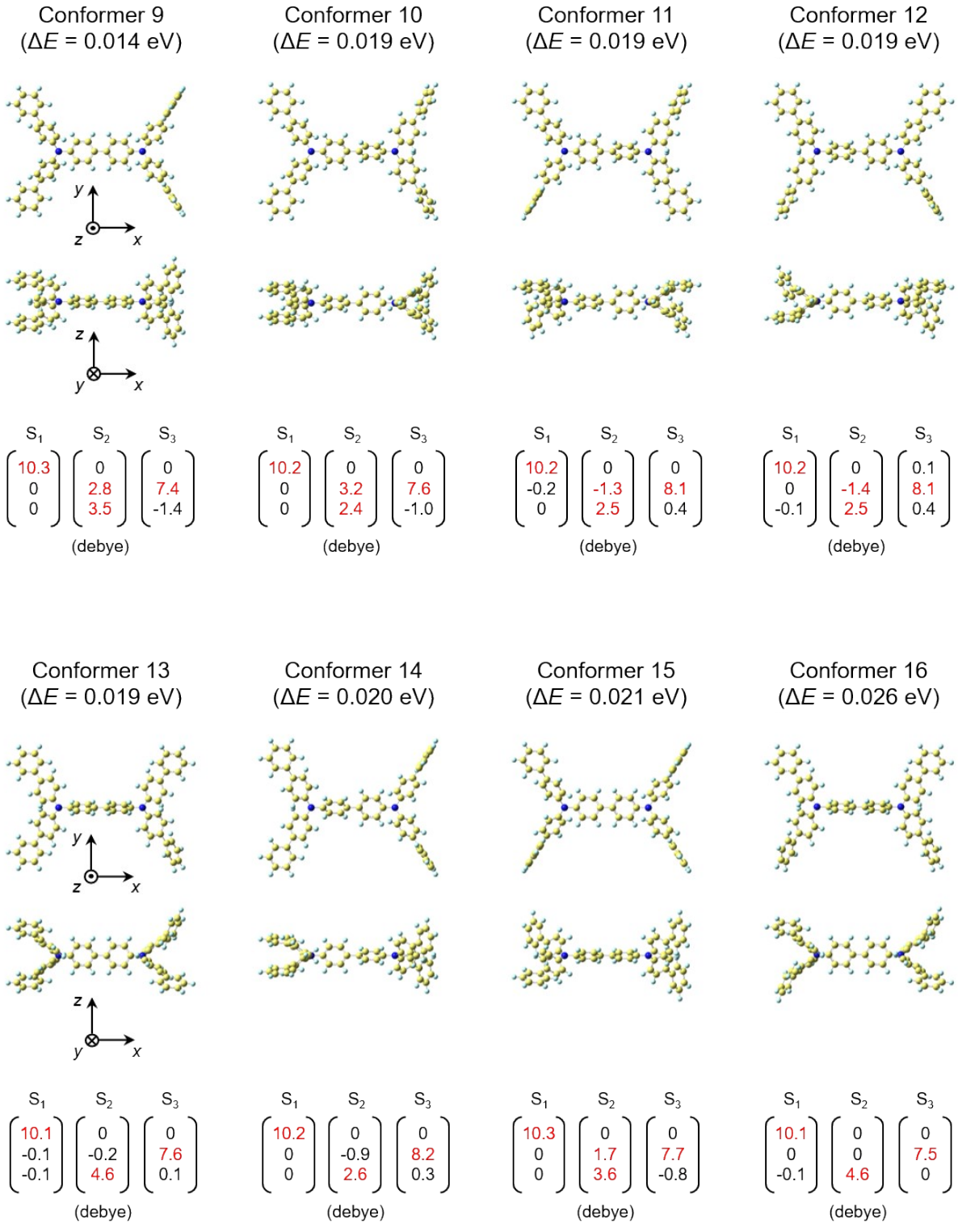

Fig. S5
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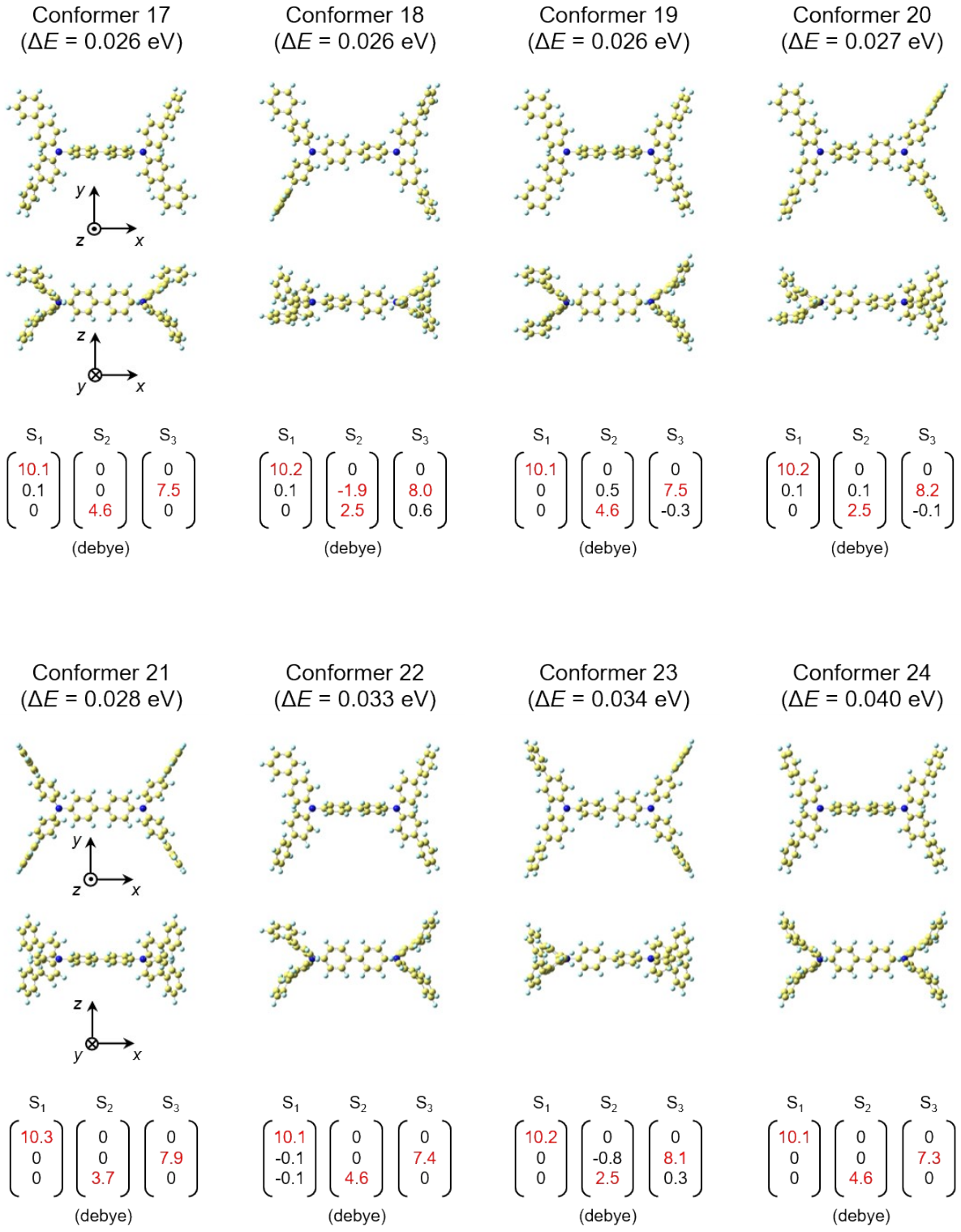

Fig. S5
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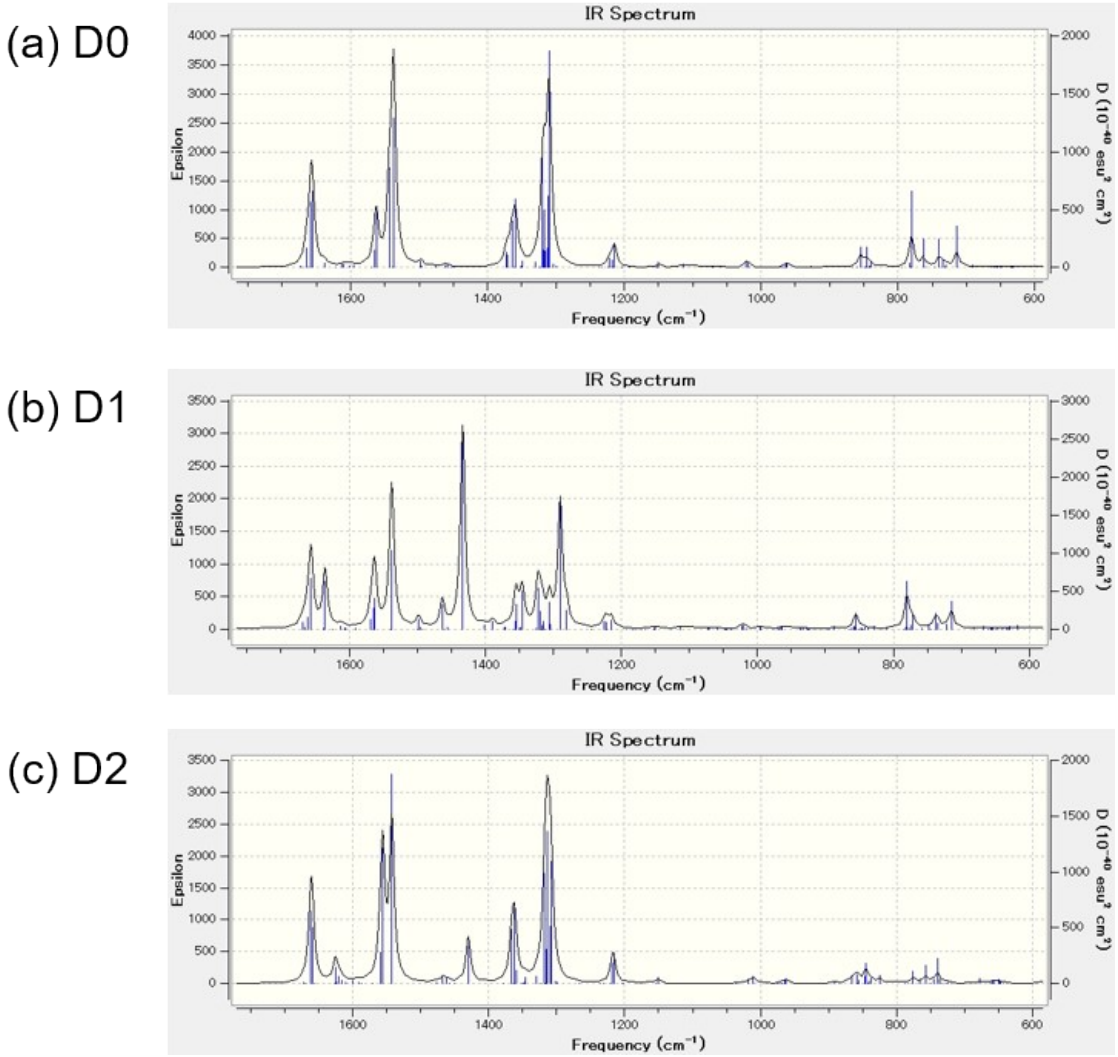

Fig. S6 Simulated IR absorption spectra of (a) BPBPA-D0, (b) D1, and (c) D2 molecules obtained by DFT B3LYP/6-31G(d) calculations.

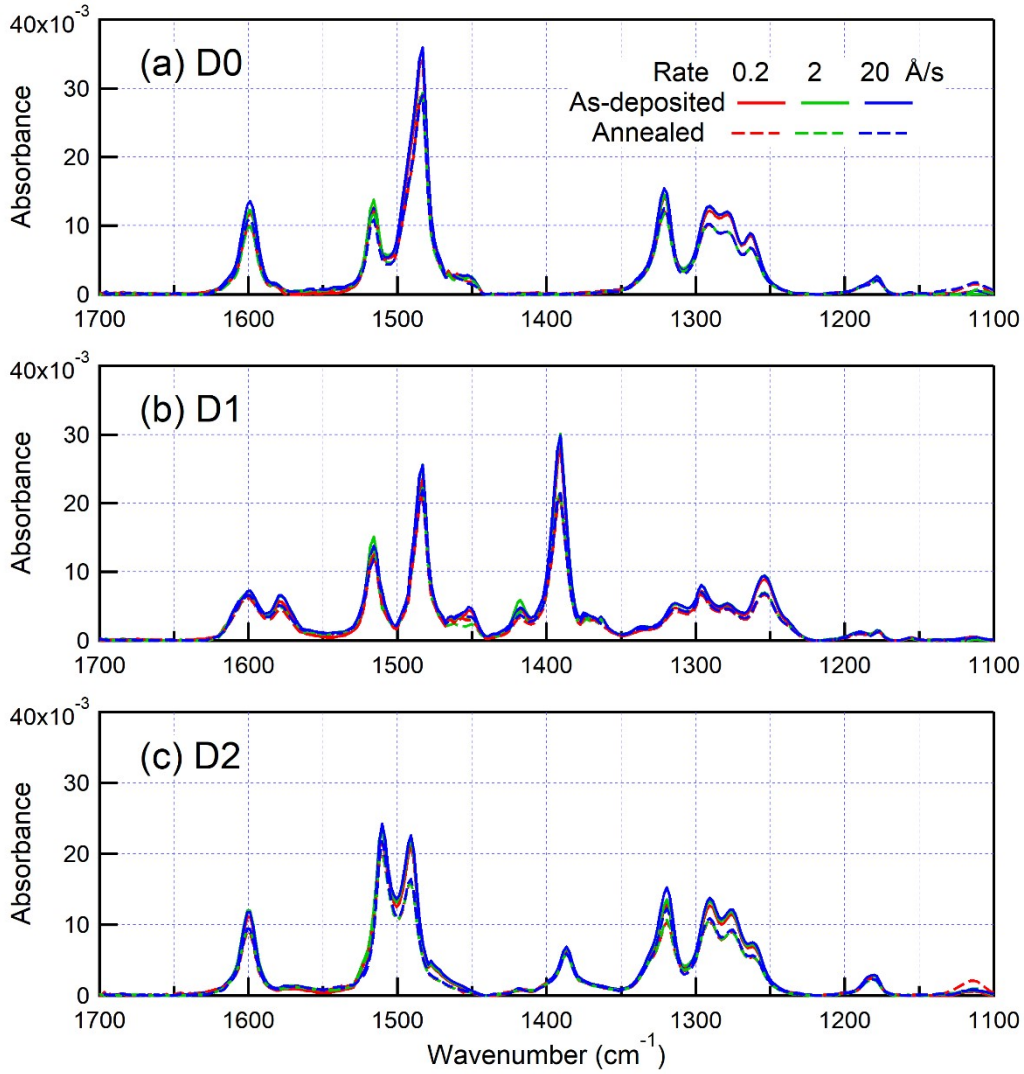

Fig. S7 Dependence of IR absorption spectra of 100-nm-thick as-deposited and annealed (a) BPBPA-D0, (b) D1, and (c) D2 films on the deposition rate in the spectral range of 1100–1700 cm^{-1}.

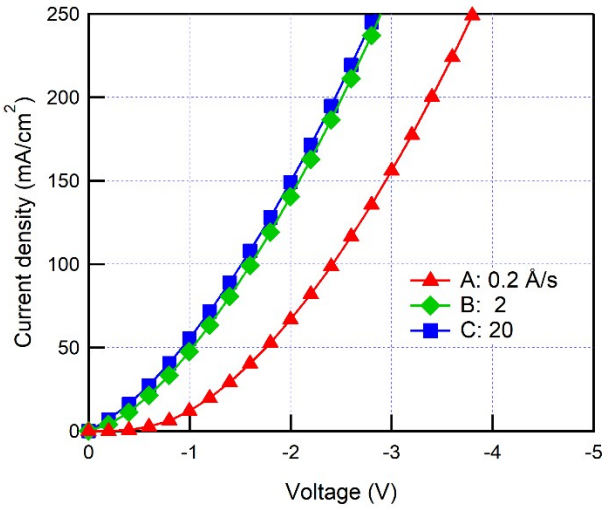

Fig. S8 *J-V* characteristics for negative voltage side of three hole-only devices A, B, and C, where BPBPA-D0 is deposited at three different deposition rates of 0.2, 2, and 20 Å s^{-1}, respectively; Device A, B, and C: glass/ITO (75 nm)/HAT-CN (5 nm)/BPBPA-D0 (100 nm at 0.2, 2, and 20 Å s^{-1})/HAT-CN (5 nm)/Au (50 nm).

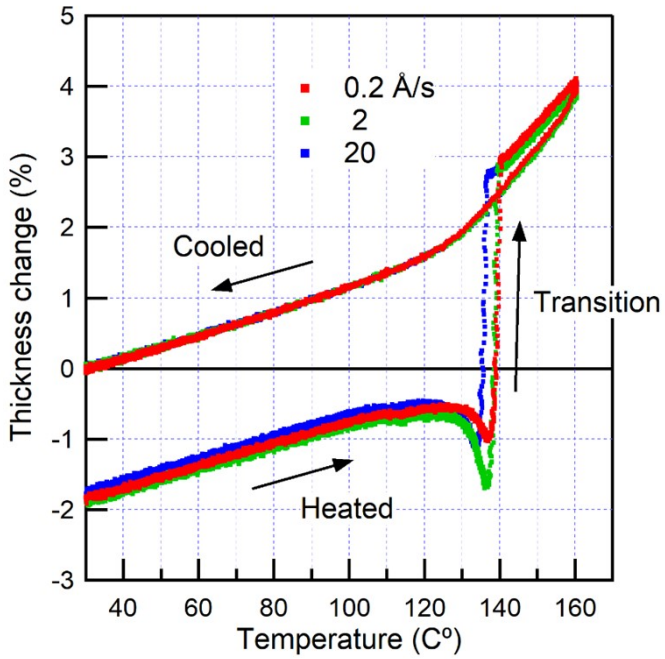

Fig. S9 Thickness changes of as-deposited BPBPA-D0 films fabricated at deposition rates of 0.2, 2, and 20 Å s^{-1} determined by *in situ* ellipsometry during a heating-cooling cycle. To compare the relative film densities of the as-deposited films, the thicknesses at 30 °C after cooling were used as the standards for normalization. The thicknesses of the as-deposited films are ~2% smaller than those of the films after cooling, but there was not a substantial difference (<0.1%) in the thickness of the as-deposited films fabricated at the different deposition rates.

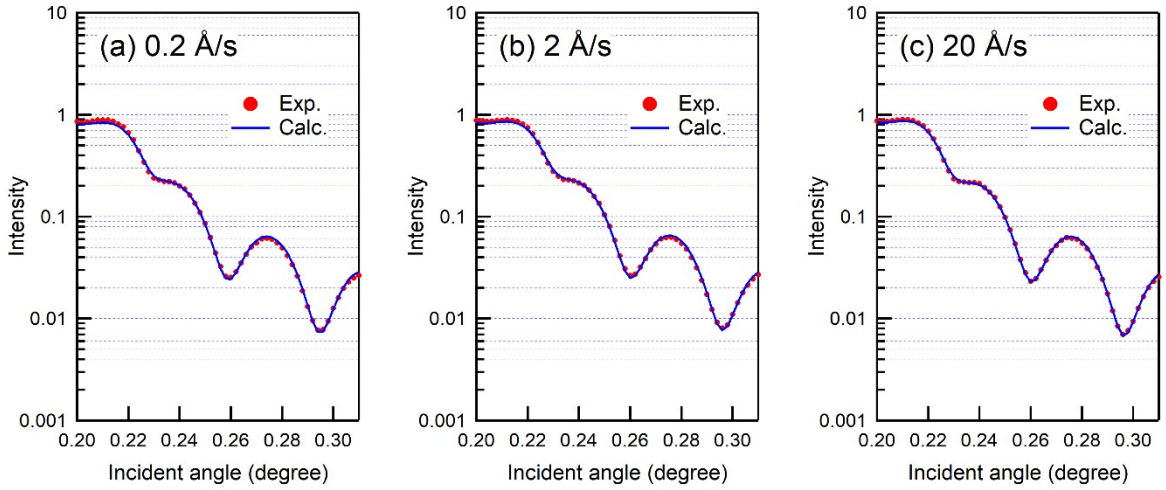

Fig. S10 XRR patterns of BPBPA-D0 films deposited on a Si(100) substrate at deposition rates of (a) 0.2, (b) 2, and (c) 20 Å s^{-1}. The analytical results of the thickness and film density are (a) 98.6 nm and 1.135 g/cm^3, (b) 98.7 nm and 1.133 g/cm^3, and (c) 97.9 nm and 1.138 g cm^{-3}.

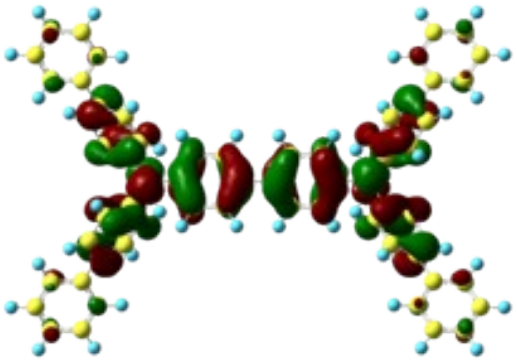

Fig. S11 Distribution of the HOMO of the BPBPA molecule obtained by DFT B3LYP/6-31G(d) calculation.

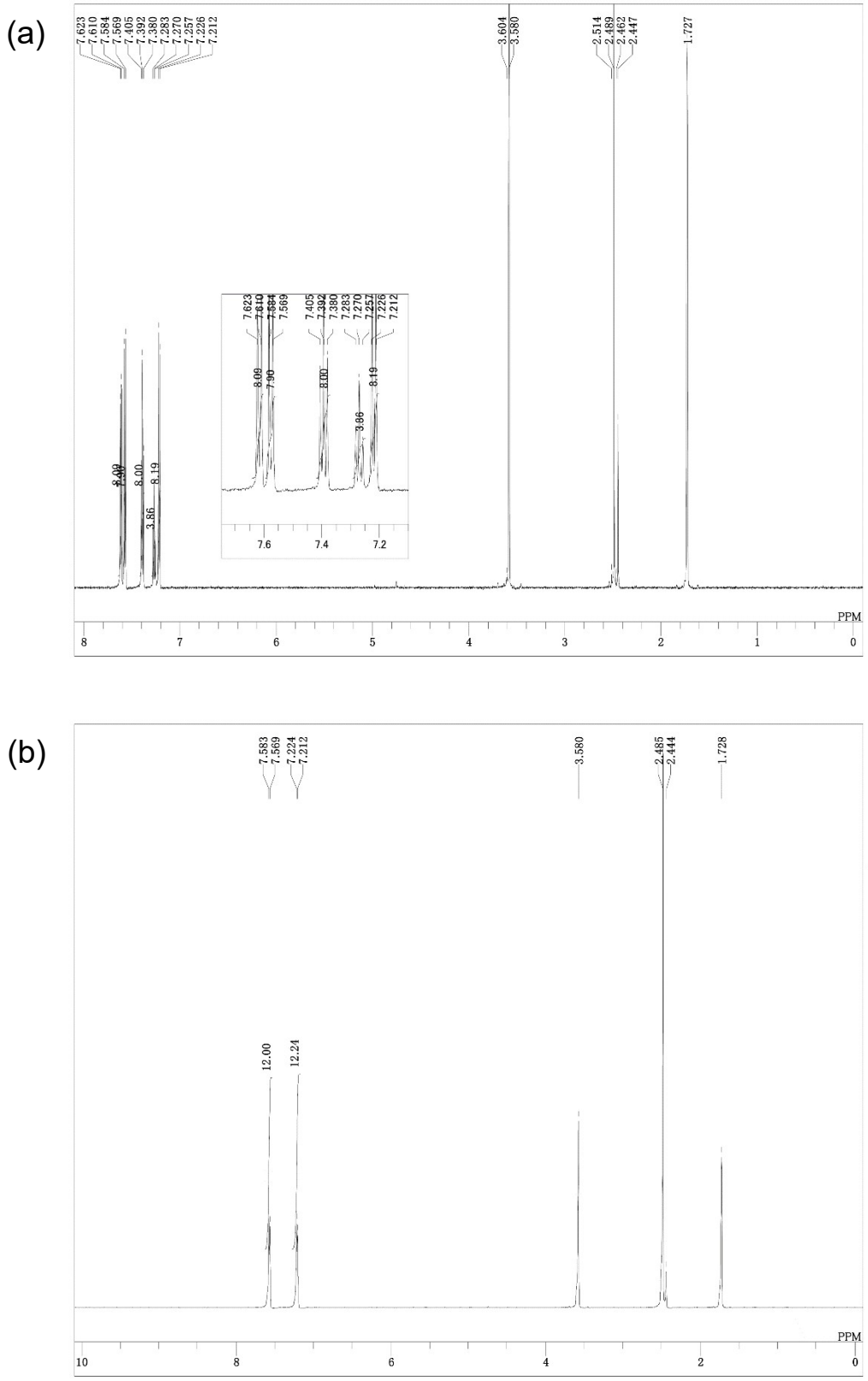

Fig. S12 [1]H-NMR spectra of (a) BPBPA-D1 and (b) D2.