

Synthesis and Configurational Character Study of Novel Structural Isomers Based on Pyrene-Imidazole

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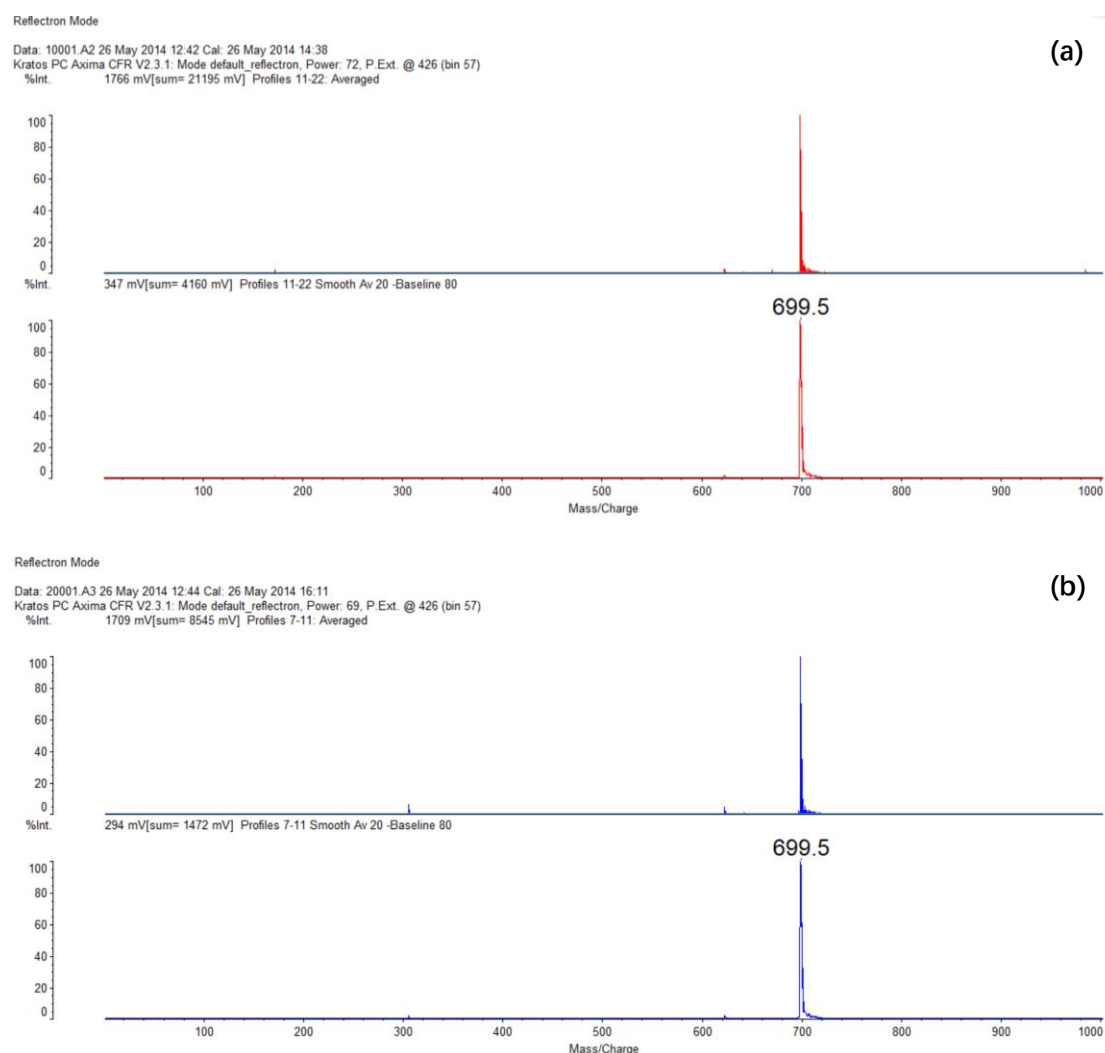


Figure S1. Mass Spectrum ($M+H^+$) of *anti*-tbu-PyDPI (a) and *syn*-tbu-PyDPI (b).

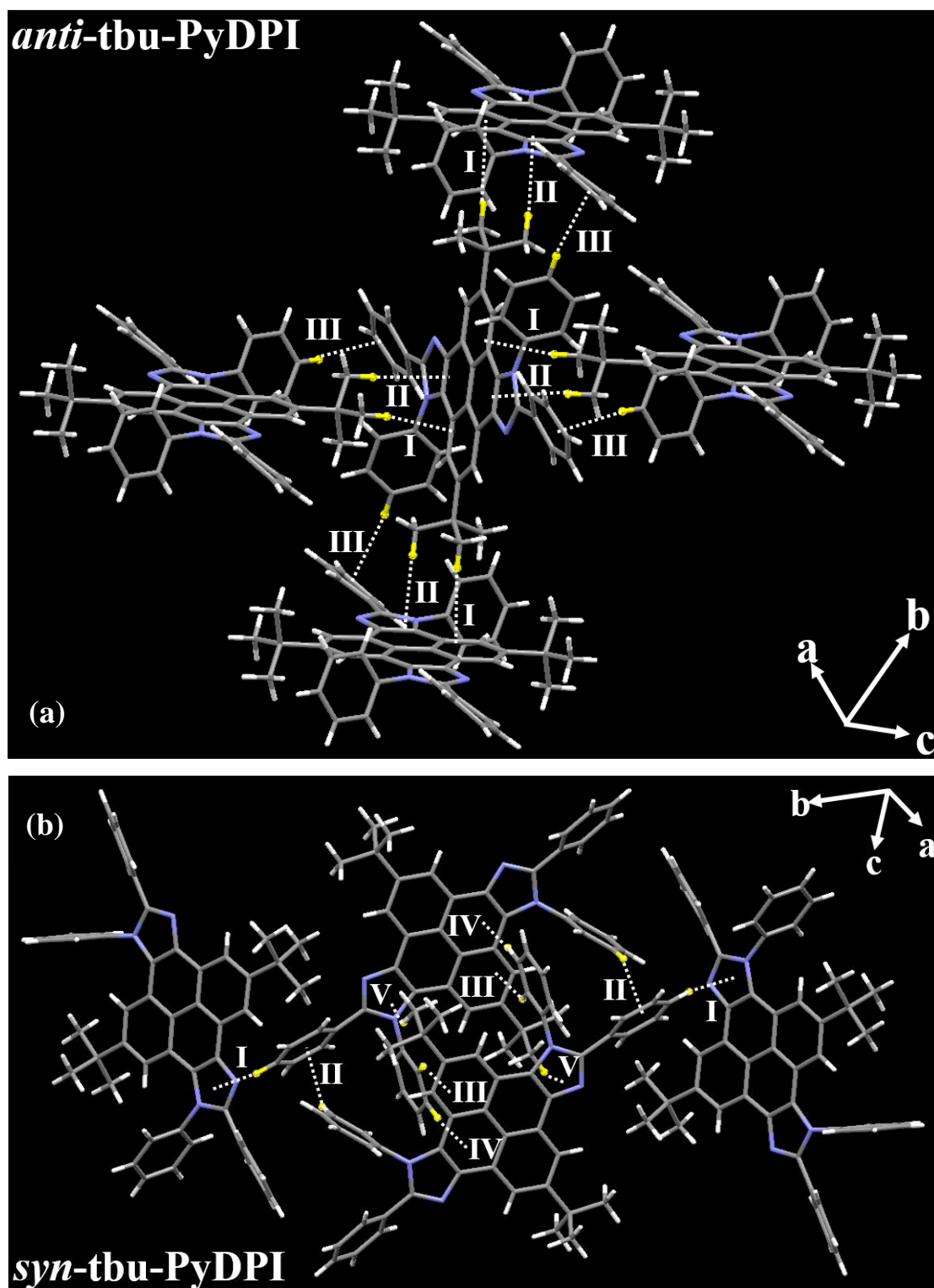


Figure S2. Packing form and the C-H... π intermolecular interactions in crystal of *anti/syn*-tbu-PyDPI.

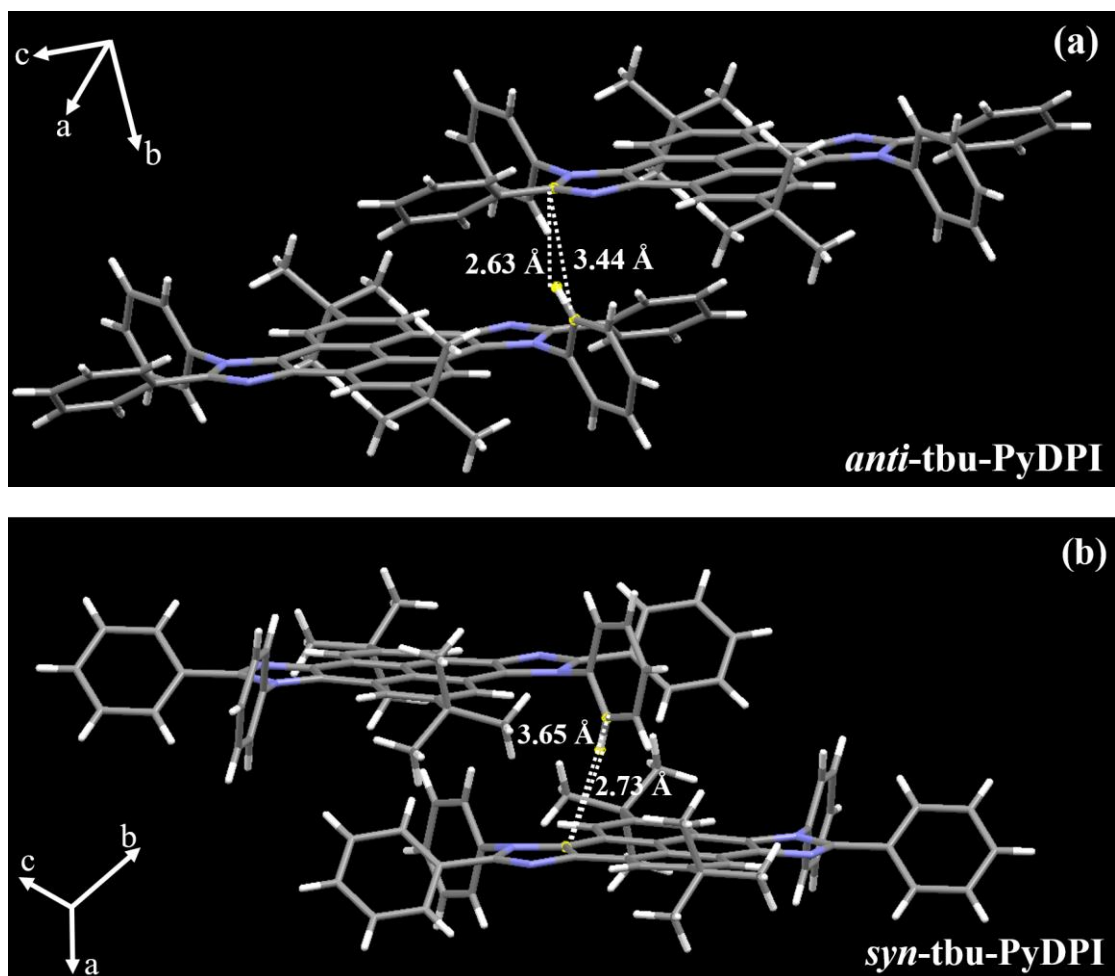


Figure S3. Short CH(sp²)···π interactions with phenyl groups at N atoms of *anti*/*syn*-*tbu*-PyDPI.

Table S1. Crystal data and structure refinements of isomers.

Compound	<i>anti</i> -tbu-PyDPI	<i>syn</i> -tbu-PyDPI
empirical formula	C ₅₀ H ₄₂ N ₄	C ₅₀ H ₄₂ N ₄
formula wt	698.88	698.88
<i>T</i> , K	296(2)	153(2)
crystal system	Monoclinic	Monoclinic
space group	P 2(1)/c	P 2(1)/c
<i>a</i> , Å	10.116(2)	11.756(2)
<i>b</i> , Å	16.062(3)	26.760(5)
<i>c</i> , Å	11.970(2)	13.272(3)
α , deg	90	90
β , deg	104.72(3)	110.23(3)
γ , deg	90	90
<i>V</i> , Å ³	1881.2(6)	3917.7(14)
<i>Z</i>	2	4
density, Mg/m ³	1.234	1.185
Absorption coefficient, mm ⁻¹	0.072	0.069
θ range, deg	3.09-25.00	3.04-25.00
no. of reflections collected	14579	27659
no. of unique reflections	3307	6875
<i>R</i> (int)	0.1546	0.0863
Good-of-fit on F ²	1.006	0.963
<i>RI</i> [<i>I</i> > 2 σ (<i>I</i>)]	0.0829	0.0578
<i>wRI</i> [<i>I</i> > 2 σ (<i>I</i>)]	0.1436	0.1473
<i>RI</i> (all data)	0.1826	0.1126