

Electronic Supporting Information (ESI)

Simple CBP isomers with high triplet energies for highly efficient blue electrophosphorescence

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Table S1 Crystal data of *o*-CBP.

<i>o</i> -CBP	
Chemical formula	C ₃₆ H ₂₄ N ₂
Formula Mass	484.57
Crystal system	monoclinic
<i>a</i> /Å	8.2215(5)
<i>b</i> /Å	18.0008(11)
<i>c</i> /Å	17.3401(11)
α ^o	90.00
β ^o	100.4060(10)
γ ^o	90.00
Unit cell volume/Å ³	2524.0(3)
Temperature/K	292(2)
Space group	<i>P</i> 2(1)/ <i>c</i>
<i>Z</i>	4
Radiation type	MoK α
μ /mm ⁻¹	0.074
<i>F</i> (000)	1016
No. of reflections measured	19886
No. of independent reflections (<i>R</i> _{int})	5503 (0.0545)
<i>R</i> (<i>F</i>), <i>wR</i> ₂ [<i>I</i> > 2 σ (<i>I</i>)]	0.0536 (0.1088)
<i>R</i> (<i>F</i>), <i>wR</i> ₂ (all data)	0.0941 (0.1220)
Goodness of fit on <i>F</i> ²	0.939
CCDC number	CCDC 846417

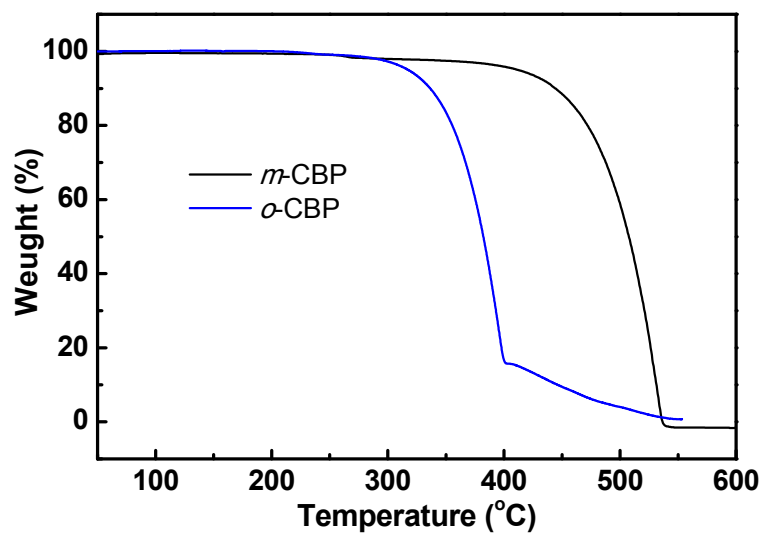


Fig. S1 TGA traces of *m*-CBP and *o*-CBP recorded at a heating rate of 10 °C min⁻¹.

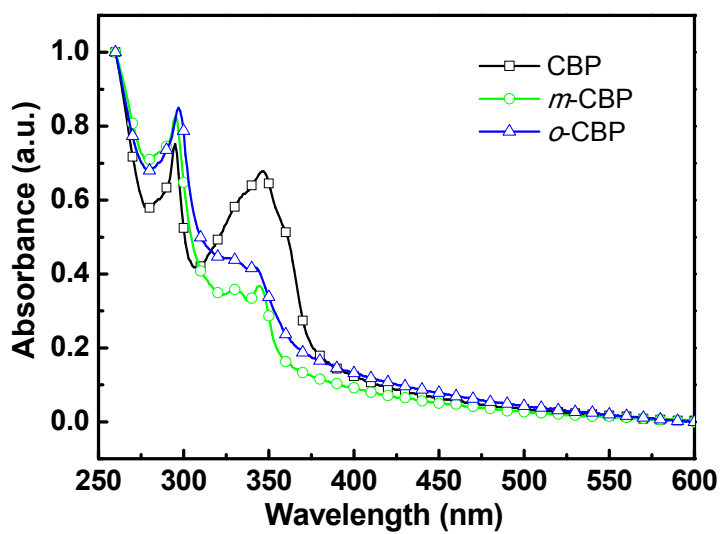


Fig. S2 UV-vis absorption of CBP, *m*-CBP and *o*-CBP in film state.