

Oxy Phosphorous Tetrabenzotriazacorrole: Firming Up the Chemical Structure and Identifying Organic Photovoltaic Functionality to Leverage Its Unique Dual Absorbance.

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Electronic Supporting Information.

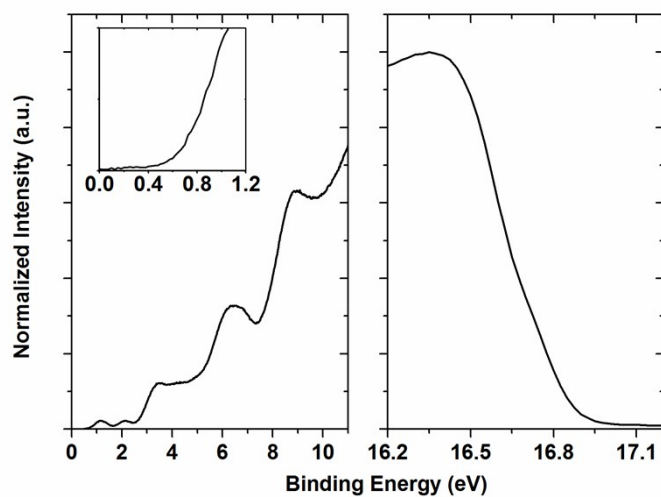


Figure S1. Ultraviolet photoelectron spectroscopy (UPS) showing the HOMO offset (left) and the secondary electron cutoff (right) of POTbc.

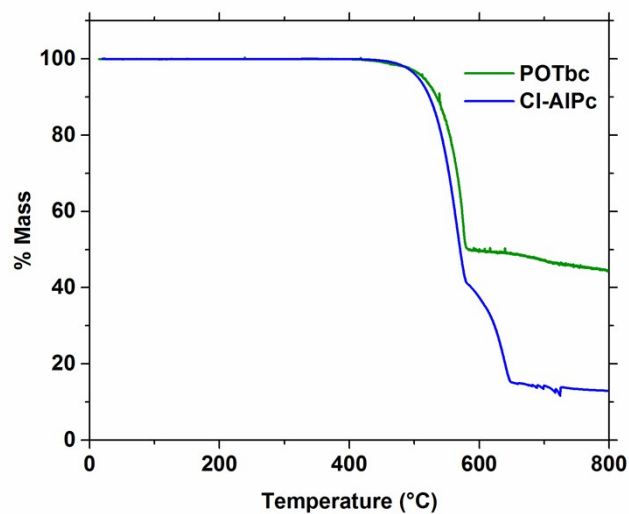


Figure S2. Thermogravimetric analysis (TGA) of POTbc and Cl-AlPc.

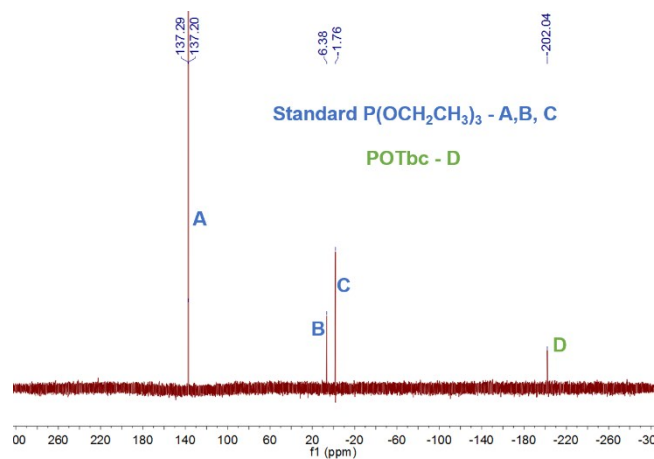


Figure S3. ^{31}P NMR spectrum of POTbc in pyridine (10% $CDCl_3$) and triethyl phosphite as a reference.

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
577 formula(e) evaluated with 11 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-3 P: 0-1

HR2-47-S11-S11 UoT GCT 17-Jun-2015
11:40:04
TOF MS E+

153617_0965 298 (4.800) Cm (251.285-92.100x0.000)

Mass	Calc. Mass	ΔPp	FW	DBE	1-FIT	Formula
345.1142	345.1141	0.1	3.2	29.5	9030.1	C26 H14 F10 F
545.1151	545.1151	0.0	3.2	29.5	15126.0	C34 H11 N3 O
545.1151	545.1151	-0.8	-1.7	32.5	14561.1	C26 H12 F6 O
545.1151	545.1151	2.2	28.3	23.5	12356.4	C32 H14 N3 O P
545.1164	545.1164	-2.2	-4.0	32.0	16382.2	C28 H15 F3 O2
545.1167	545.1167	3.5	4.8	28.5	11617.9	C34 H13 F4 O2
545.1174	545.1174	2.6	3.1	25.0	6256.8	C22 H16 F9 O3
545.1174	545.1174	5.1	5.7	26.5	9722.8	C31 H13 F3 O3
545.1178	545.1178	-2.6	-6.0	32.5	17629.1	C45 H17 O5
545.1181	545.1181	3.9	7.2	28.0	13376.1	C38 H20 F4 O3
545.1195	545.1195	4.7	8.6	32.5	17241.7	C45 H18 O F

Figure S4. High resolution mass spectrum of POTbc.