Supporting information

A Perylene Diimide Crystal with High Capacity and Stable Cyclability for Na-ion Batteries

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1. Table S1. Crystal data of PTCDI*

Emperical formula	$C_{24}H_{10}O_4N_2$
Formula weight	390
Temperature	263.2K
Crystal system, space group	Monoclinic, P 21/n
Symmetry Int-Tables number	14
Unit cell dimensions	a= 4.865(4) Å, b=14.660(7) Å, c=10.844(3) Å, α =90°,β=91.33(4)°,γ = 90°
Volume	773.195
Z, Calculated density	2, 1.677
R-Factor	7.04%

* The crystal information file (CIF) of PTCDI is available from The Cambridge Crystallographic Data Centre (CCDC) software (http:// www.ccdc.cam.ac.uk).[1]

2. Table S2. ICP results of Na^+ content in PTCDI electrodes at different potential states

Charge/discharge states	Na^+ content (wt.%) in Na_x[PTCDI]	Corresponding n(Na^+) per PTCDI unit
Discharge to 2.0 V	4.77	0.85
Discharge to 1.75 V	6.30	1.14
Discharge to 1.0 V	10.48	1.98
Charge to 2.2 V	6.09	1.1
Charge to 2.6 V	4.5	0.8
Charge to 3.0 V	0.07	0

1. Groom, C. R.; Allen, F. H., The Cambridge Structural Database in Retrospect and Prospect. *Angewandte Chemie International Edition* **2014,** *53* (3), 662-671.