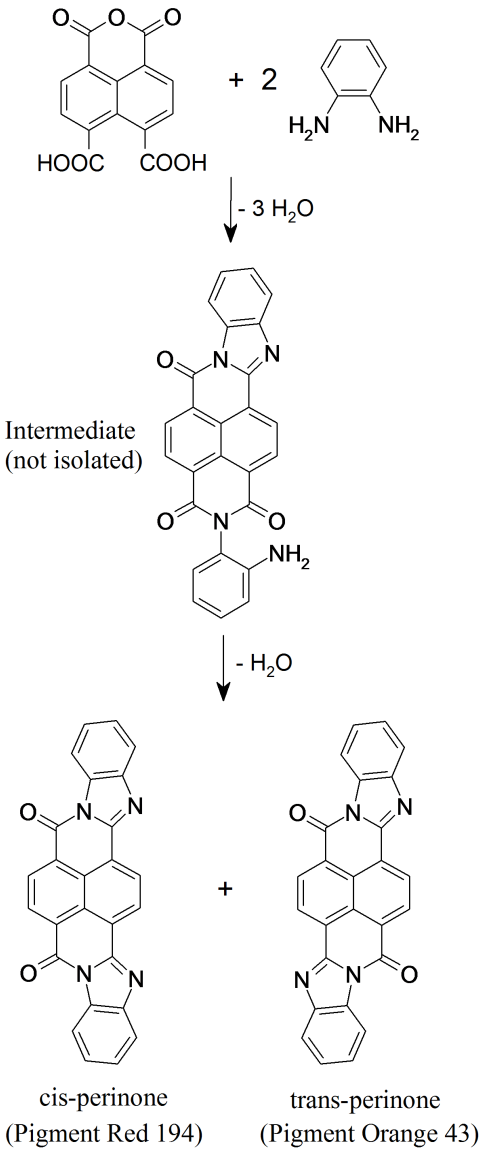
STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 75 (2019)

Supporting information for article:

Two new polymorphs of *cis*-perinone: crystal structures, physical and electric properties

D. A. Zherebtsov, M. U. Schmidt, R. Niewa, C. P. Sakthidharan, F. V. Podgornov, Y. V. Matveychuk, S. A. Nayfert, M. A. Polozov, S. N. Ivashevskaya, A. I. Stash, Yu-Sheng Chen, D. E. Zhivulin, V. E. Zhivulin, S. V. Merzlov, E. V. Bartashevich, V. V. Avdin, Hua Shu Hsu and Feng Wei Guo



Scheme S1: Synthesis of perinones

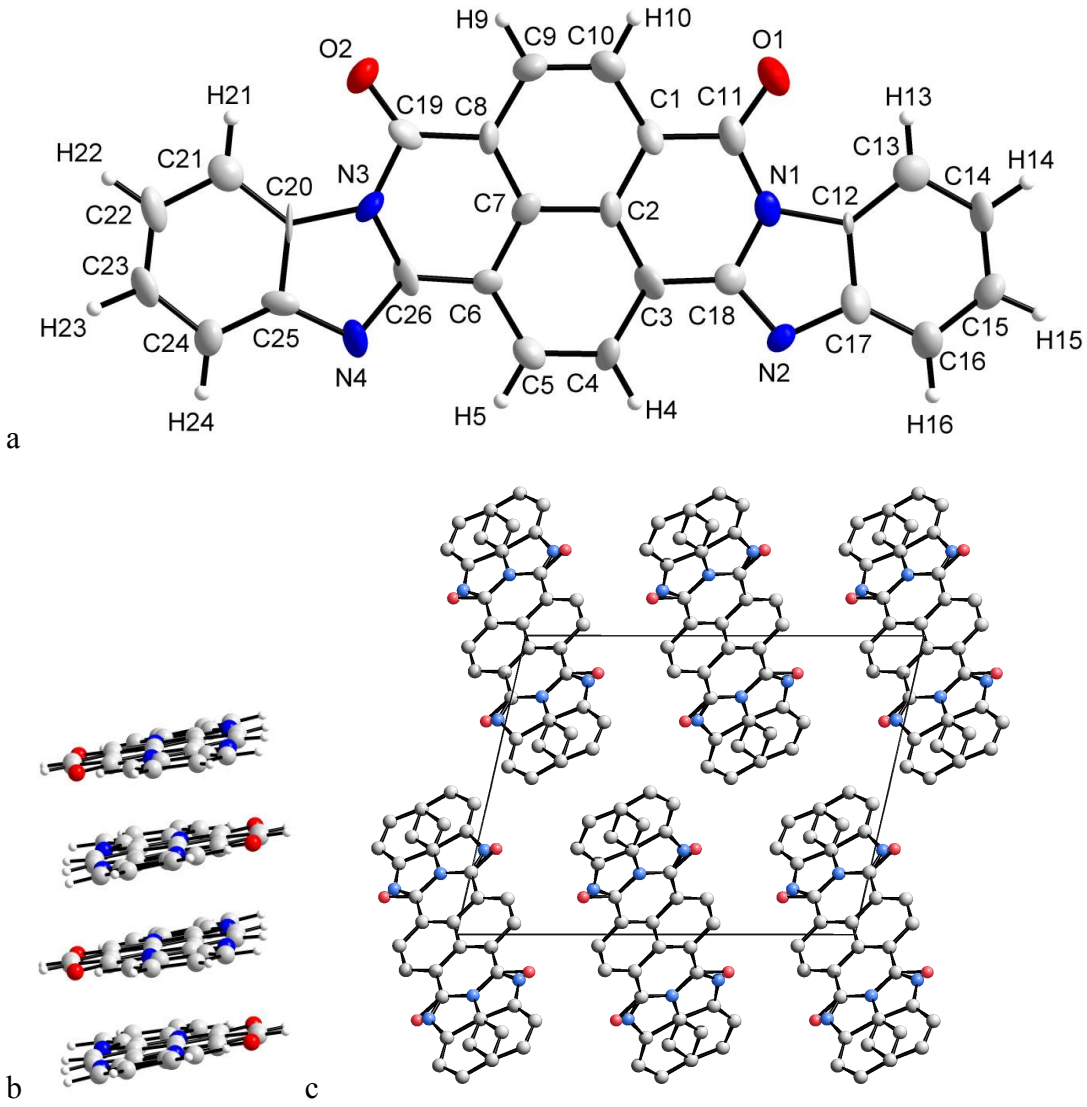


Figure S1 Crystal structures of *cis*-perinone polymorphs. (a) single molecule in phase **2**; (b) **2**, orientation of the molecules within a stack; (c) disordered polymorph, view along the *b* axis (Mizuguchi, 2003a).

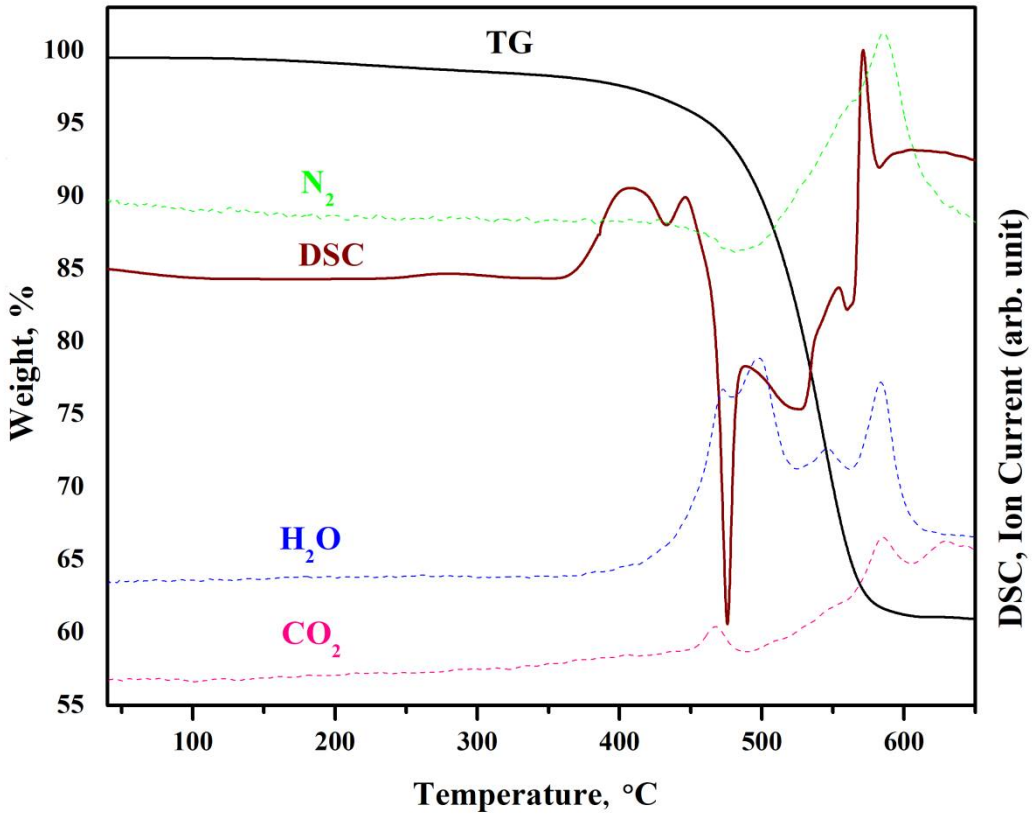


Figure S2 The results of simultaneous TG-DSC-QMS analysis of **2**

Table S1 Assigned IR frequencies for crystal **1** (cm^{-1})

Vibration assignments	Calculated IR frequencies	Experimental IR frequencies
$\nu_{C–H}$ (benzene ring)	3136s, 3131s, 3118s, 3099s, 3081s, 3064s	3103w, 3071w, 3053w, 3019w
$\nu_{C=O}$	1718m	1697ss
		1609m
$\nu_{C–C–C}$ asym (benzene ring)	1607w	
$\nu_{C–C}$ (benzene ring)	1598w, 1589w, 1504m	1580m, 1499w
$\nu_{C–C}$ (benzene ring), $\nu_{C–C–C}$ asym (benzene & pyridine ring)	1577w	
$\nu_{C–C=N}$ asym (pyridine & imidazole ring)	1548w	1541m
		1477w
$\nu_{C–C–C}$ sym (benzene ring), $\delta_{H–C–C-H}$ rock (benzene ring)	1465s	1447s
$\nu_{C–C–C}$ sym (benzene ring), $\nu_{C–C=N}$ sym (pyridine & imidazole ring)	1411w	1402m
$\nu_{C–C–C}$ sym (benzene ring), $\nu_{C–C–C}$ asym (benzene ring), $\nu_{C–C–C}$ asym (pyridine ring), $\nu_{C–C–N}$ asym (pyridine ring)	1395m	
$\nu_{C–C–C}$ asym (benzene ring), $\nu_{C–C–N}$ asym (pyridine ring)	1390m	1383s
$\nu_{C–C–C}$ asym (benzene ring)	1365w	1352s
$\delta_{H–C–C-H}$ sciss (benzene ring), $\delta_{H–C–C-H}$ rock (benzene ring), $\nu_{C–C–C}$ asym (benzene & pyridine ring), $\nu_{N=C–N}$ asym (imidazole ring)	1303s	1304m
		1288m
$\delta_{H–C–C-H}$ rock (benzene ring), $\nu_{C–C–C}$ sym (benzene ring)	1276m	1273m
$\delta_{H–C–C-H}$ sciss (benzene ring), $\nu_{C–C–C}$ sym (benzene ring)	1233m	1225m
		1179m
$\delta_{H–C–C-H}$ sciss (benzene ring), $\nu_{C–C–C}$ sym (benzene ring), $\nu_{C–N–C}$ asym (pyridine ring)	1172w	
$\delta_{H–C–C-H}$ sciss (benzene ring)	1137w, 1132w	1134m
$\delta_{H–C–C-H}$ sciss (benzene ring), $\delta_{H–C–C-H}$ rock (benzene ring)	1127m, 1103s, 1082w, 1021m	1101w, 1009w
$\delta_{H–C–C-H}$ sciss (benzene ring), $\nu_{C–N–C}$ asym (pyridine ring)	1121m	
$\delta_{H–C–C-H}$ sciss (benzene ring), $\nu_{C–C–N}$ sym (pyridine ring)	1120m	
$\delta_{H–C–C-H}$ rock (benzene ring), $\delta_{H–C–C-H}$ sciss (benzene ring)	1003m	991m
$\gamma_{H–C–C-H}$ twist (benzene ring)	954w, 919w	941w, 903w
$\gamma_{H–C–C-H}$ twist (benzene ring), $\gamma_{H–C–C-H}$ wagg (benzene ring)	876m	878m
$\gamma_{H–C–C-H}$ wagg (benzene ring), $\gamma_{H–C–C-H}$ twist (benzene ring)	872w, 862m, 852m	860m

$\gamma_{H–C–C-H}$ wagg (benzene ring)	840s, 837s, 834w	
		793w
$\gamma_{H–C–C(H)–C–H}$ wagg (benzene ring)	756ss	758ss
$\gamma_{H–C–C(H)–C–H}$ wagg (benzene ring), Γ (pyridine ring)	743m	
$\gamma_{H–C–C(H)–C–H}$ wagg (benzene ring), Γ (pyridine & imidazole ring)	737m	
$\gamma_{H–C–C(H)–C–H}$ wagg (benzene ring), Δ (benzene ring), Γ (imidazole ring)	729w	
$\gamma_{H–C–C–H}$ wagg (benzene ring), Γ (pyridine ring)	715m	704w
Δ (benzene ring)	627s	621m
Γ (benzene & pyridine ring)	597m, 466w, 461w, 442m	594w, 463m, 438w
Δ (benzene & pyridine ring)	586m, 516s, 456w	511w
		494w

Description of assignment: ν – stretching (symmetric & asymmetric), δ – in-plane bending (scissoring & rocking), γ – out-of-plane bending (twisting & wagging), Γ – out-of-plane ring deformation, Δ – in-plane ring deformation. The relative intensity: w – weak, m – medium, s – strong, ss – super-strong.