Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

for

New Acentric Quinolinium Crystal with High Order Parameter for Nonlinear Optical and Electro-Optic Applications

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1. Crystallographic Data

Table S1. X-ray data collection and structure refinement for HMQ-NS.

Empirical formula	$C_{29}H_{25}NO_5S$	μ, mm^{-1}	0.183
Formula weight	499.56	F(000)	524
Temperature, K	296(2)	T_{max}	0.9712
Crystal system	monoclinic	T_{min}	0.9573
Space group	*Pn*	θ range (º)	2.32–28.43
a, Å	7.1438(2)	No. of reflns collected	17297
b, Å	10.8234(2)	No. of reflns independent	5202
c, Å	15.2054(3)	No. of reflns with $I > 2\sigma(I)$	4274
α, (º)	90	No. of parameters	402
β, (º)	99.5620(10)	Flack parameter	0.04(6)
γ, (º)	90	Max., in $\Delta\rho$ (e Å^{-3})	0.221
V, Å^3	1159.35(5)	Min., in $\Delta\rho$ (e Å^{-3})	−0.194
Z	2	*GOF* on F^2	1.042
d_{cal}, g cm^{-3}	1.431	R^a	0.0394
		$wR2^b$	0.0851

$^aR = \Sigma[|F_o| - |F_c|]/\Sigma|F_o|]$, $^bwR2 = \Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]^{1/2}$

Table S2. Selected bond lengths (Å) and bond angles (º) in HMQ-NS crystal.

S1–O4	1.442(2)	S1–O5	1.444(2)	S1–O3	1.455(2)
O1–C14	1.365(3)	O1–C18	1.412(3)	O2–C15	1.345(3)
N1–C19	1.484(3)				
O4–S1–O5	114.3(1)	O4–S1–O3	113.3(1)	O5–S1–O3	112.7(1)
C14–O1–C18	118.6(2)	N1–C1–S1	179.6(2)	C2–C3–C4	178.6(3)

Table S3. Hydrogen bonds for HMQ-NS crystal (Å and °).

D–H···A	D–H	H···A	D···A	D–H–A
O2–H2O···O1	0.82(4)	2.28(4)	2.667(2)	109(3)
O2–H2O···O3	0.82(4)	1.90(4)	2.664(2)	155(4)

2. Quantum Chemical Calculations

Table S4. Calculated results of the finite-field (FF) method with the experimental (EXP) cation structures of HMQ-NS and HMQ-T crystals at the B3LYP/6-311+G(d) level: the zero-frequency hyperpolarizability tensor β_{ijk} ($\times 10^{-30}$ esu) and the first-order hyperpolarizability β_{max} ($\times 10^{-30}$ esu).

	HMQ-NS cation (EXP)	HMQ-T cation (EXP) [14]
β_{xxx}	0.42	0.23
β_{xxy}	-0.38	-0.27
β_{xyy}	0.12	0.15
β_{yyy}	-0.37	-0.32
β_{xxz}	2.34	1.32
β_{xyz}	-1.53	-1.02
β_{yyz}	0.05	0.88
β_{xzz}	15.15	8.44
β_{yzz}	-14.89	-19.43
β_{zzz}	155.92	164.95
β_{max}	160.3	169

Table S5. The components of β_{ijk}^{eff} tensor (in 10^{-30} esu) in the Cartesian *XYZ* system.

	β_{333}^{eff}	β_{223}^{eff}	β_{113}^{eff}	β_{111}^{eff}	β_{221}^{eff}	β_{331}^{eff}
HMQ-NS	**-149.4**	-5.8	-0.8	0.0	-0.1	0

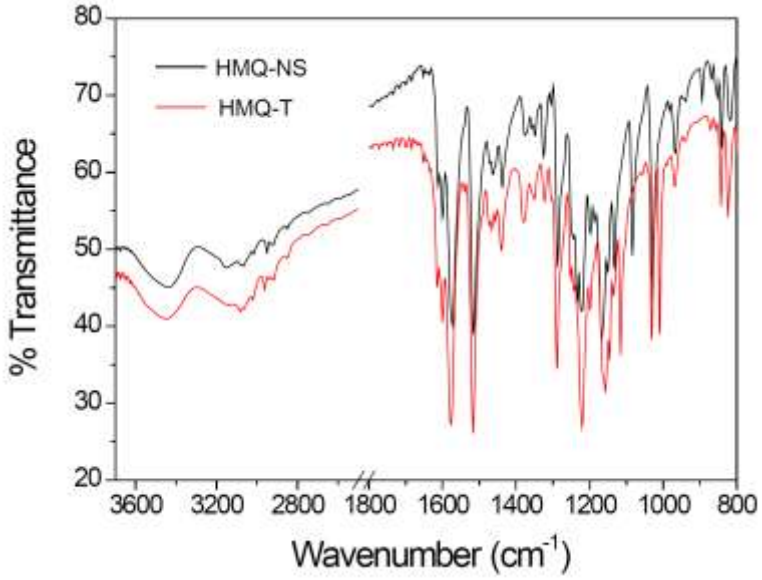

Figure S1. Infrared (IR) absorption spectra of HMQ-NS and HMQ-T[14] crystals.

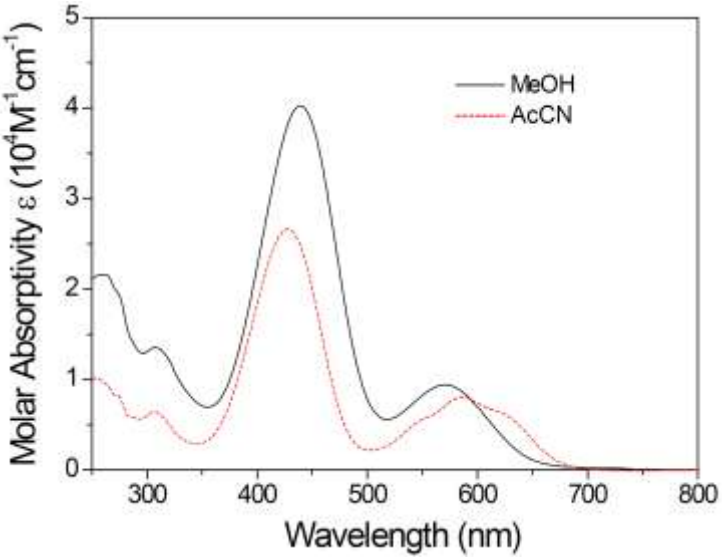

Figure S2. UV-vis. absorption spectra of HMQ-NS compound in methanol and acetonitrile solutions.