

Supplementary Materials

Organic nonlinear optical crystals for highly efficient terahertz-wave generation

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Table S1. The compounds mentioned in different structure series.

Series	Chemical Structure		Full names of crystals
Pyridinium-based		DAST ²⁰ (C ₂₃ H ₂₆ N ₂ O ₃ S)	4-Dimethylamino-N-methyl-4-stilbazolium tosylate
		OHP-TFS ²⁸ (C ₂₁ H ₁₈ NO ₄ F ₃ S)	4-(4-hydroxystyryl)-1-methylpyridinium-1-ium 4-(trifluoromethyl)benzenesulfonate
		DHP-TFS ³³ (C ₂₁ H ₁₈ NO ₅ F ₃ S)	4-(3,4-Dihydroxystyryl)-1-methylpyridinium 4-(trifluoromethyl)benzenesulfonate
Quinolinium-based		HMQ-T ³⁸ (C ₂₆ H ₂₅ NO ₅ S)	2-(4-hydroxy-3-methoxystyryl)-1-methylquinolinium 4-methylbenzenesulfonate
		HMQ-4TFS ²⁹ (C ₂₆ H ₂₂ F ₃ NO ₅ S)	2-(4-hydroxy-3-methoxystyryl)-1-methylquinolinium 4-(trifluoromethyl)benzenesulfonate
		OHQ-T ⁴⁰ (C ₂₅ H ₂₃ NO ₄ S)	2-(4-hydroxystyryl)-1-methylquinolinium 4-methylbenzenesulfonate
		OHQ-CBS ⁴⁴ (C ₂₄ H ₂₀ ClNO ₄ S)	2-(4-hydroxystyryl)-1-methylquinolinium 4-chlorobenzenesulfonate
		OHQ-TFO ⁴⁵ (C ₂₅ H ₂₀ F ₃ N ₅ O)	2-(4-hydroxystyryl)-1-methylquinolinium 4-(trifluoromethoxy)benzenesulfonate
		HM7CIQ-CBS ⁴² (C ₂₅ H ₂₁ Cl ₂ NO ₅ S)	7-chloro-2-(4-hydroxy-3-methoxystyryl)-1-methylquinolinium 4-chlorobenzenesulfonate
		HM6FQ-T ⁴³ (C ₂₆ H ₂₄ FNO ₅ S)	6-fluoro-2-(4-hydroxy-3-methoxystyryl)-1-methylquinolinium 4-methylbenzenesulfonate
		HM7CIQ-T ⁴² (C ₂₆ H ₂₄ ClNO ₅ S)	7-chloro-2-(4-hydroxy-3-methoxystyryl)-1-methylquinolinium 4-methylbenzenesulfonate
Benzothiazolium-based		PMB-T ⁴⁶ (C ₂₉ H ₃₂ N ₂ O ₄ S ₂)	2-(4-(4-(hydroxymethyl)piperidin-1-yl)styryl)-3-methylbenzo[d]thiazol-3-ium 4-methylbenzenesulfonate

Series	Chemical Structure		Full names of crystals
Benzothiazolium-based		HMB-TMS ⁴⁷ (C ₂₆ H ₂₇ NO ₅ S ₂)	2-(4-hydroxy-3-methoxystyryl)-3-methylbenzo- [d]thiazol-3-ium 2,4,6-trimethylbenzenesulfonate
		HDB-T ⁴⁸ (C ₂₅ H ₂₅ NO ₄ S ₂)	2-(4-hydroxy-3,5-dimethylstyryl)-3-methylbenz- o[d]thiazol-3-ium 4- methylbenzenesulfonate
		OHB-TFO ⁴⁹ (C ₂₃ H ₁₈ F ₃ NO ₅ S ₂)	2-(4-hydroxystyryl)-3-methylbenzothiazol-3-ium 4-(trifluoromethoxy)benzenesulfonate
		PFB-CBS ⁵⁰ (C ₂₈ H ₂₈ ClFN ₂ O ₄ S ₂)	5-fluoro-2-(4-(4-(hydroxymethyl)piperidin-1- yl)styryl)-3-methylbenzothiazol-3-ium 4-chlorobenzenesulfonate
		PMB-4TFS ²⁷ (C ₂₉ H ₂₉ N ₂ O ₄ S ₂ F ₃)	2-(4-(4-(hydroxymethyl)piperidin-1-yl)styryl)-3- methylbenzothiazol-3-ium 4-(trifluoromethyl) benzenesulfonate
		PMB-TFO ⁵¹ (C ₂₉ H ₂₉ N ₂ O ₅ S ₂)	2-(4-(4-(hydroxymethyl)piperidin-1-yl)styryl)-3- methylbenzothiazol-3-ium 4-(trifluoromethoxy)benzenesulfonate
Indolium-based		EHPSI-4NBS ⁵² (C ₃₂ H ₃₇ N ₃ O ₆ S)	(E)-1-ethyl-2-(4-(4-(hydroxymethyl)piperidin-1- yl)styryl)-3,3-dimethyl-3H-indol-1-ium 4-nitrobenzenesulfonate
		OHI-T ⁵³ (C ₂₆ H ₂₇ NO ₄ S)	2-(4-hydroxy)styryl-1,3,3-trimethylindolenium 4-methylbenzenesulfonate
Benzoindolium-based		P-BI ⁵⁴ (C ₂₅ H ₂₇ IN ₂)	(E)-2-(4-(dimethylamino)styryl)-1,1,3-trimethyl- 1H-benzo[e]indol-3-ium iodide
		MBI ⁵⁵ (C ₂₄ H ₂₄ NOI)	(E)-2-(4-(Methoxy)styryl)-1,1,3-trimethyl-1H- benzo[e]indol-3-ium iodide
Benzimidazolium-based		HMI-TMS ⁵⁶ (C ₂₇ H ₃₀ N ₂ O ₅ S)	2-(4-hydroxy-3-methoxystyryl)-1,3-dimethyl-1H- benzimidazol-3-ium 2,4,6-trimethylbenzenesulfonate