Supporting Information (SI)

Synthesis and characterization of a new isoxazolone-based nonlinear optical crystal: MPMOI

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Contents.

1. Supplementary Figures.

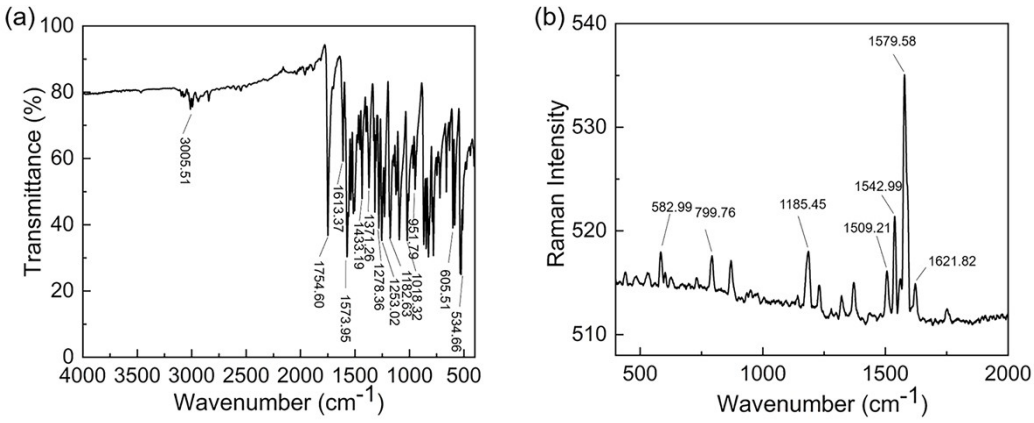


Figure. S1. (a) FT-IR and (b) Raman spectrum of MPMOI.

Reported

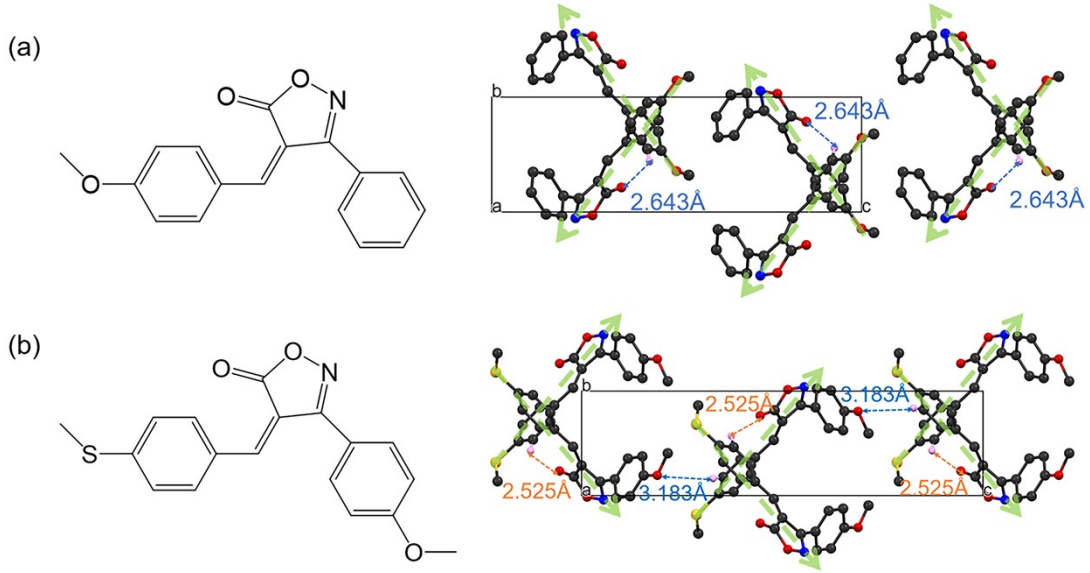


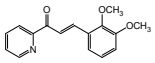
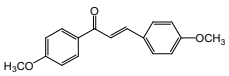
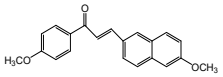
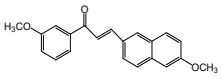
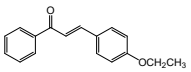
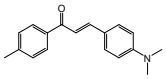
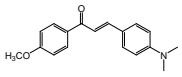
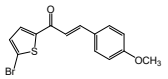
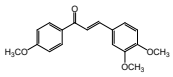
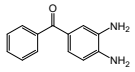
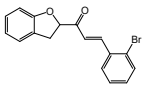
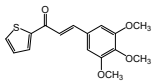
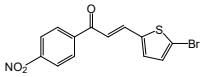
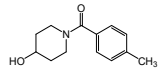
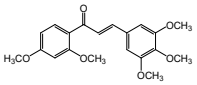
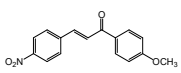
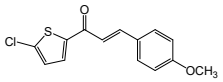
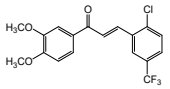
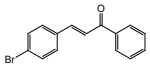
Figure. S2. Chemical structures and hydrogen contacts in (a) MLS and (b) MPMI viewed down along *a* axis.

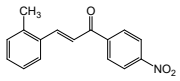
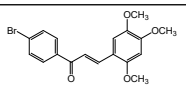
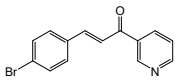
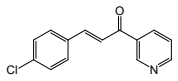
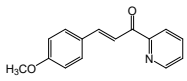
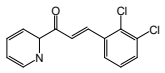
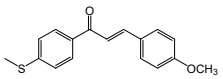
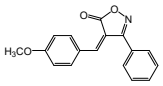
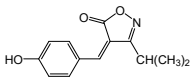
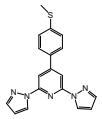
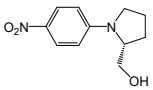
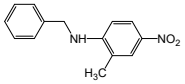
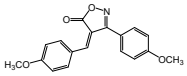
2. Supplementary Tables.

Table S1. The vibration modes of MPMOI.

$\upsilon_{FT\text{-}IR}$ (cm^{-1})	υ_{Raman} (cm^{-1})	Assignment
534.66, 605.51		Deformation vibration of benzene ring[S1]
	799.76	Symmetric vibration of C-O-C
951.79		$=CH_2$ oscillates out of the plane
1018.32		C-O link to the alkyl group stretches
1182.63		CH_2 wobbles out of the face
	1185.45	CH_3 out-of-plane bending[15]
1253.02，1278.36		Stretching vibration of aromatic ring C-C
1371.26		Bending vibration of methyl groups[S1]
1433.19		Symmetrical bending vibrations of alkyl group (CH_3-) [S2]
1573.95		Aromatic ring skeleton vibration
	1509.28, 1542.99	C=C bonds
	1579.58	Aromatic ring C-C bond
1754.60, 1613.37		Stretching vibration of C=O [S2]
3005.51		C-H stretching of aromatic ring[S3]

Table S2. SHG properties of organic nonlinear optical crystals with similar ketone – methoxy group structures and the crystals mentioned in the article.

Crystal Name	Chemical Structure	Space Group	SHG *	Melting point	Ref.
DMPP		Orthorhombic $P\text{ca}2_1$	≈ KDP	80	54
BMP		Orthorhombic $P2_12_12_1$	1.04 × urea	107	55
6MN4MPP		Monoclinic $P\text{n}$	2.18 × KDP	137.4	15
6MN3MPP		Orthorhombic $P\text{ca}2_1$	4.3 × KDP	131.7	15
EBC		Monoclinic $P2_1$	20 × KDP	127.45	S4
DAMC		Orthorhombic $P2_12_12_1$	0.8 × urea	-	51,52
DAMO		Monoclinic $P2_1$	42.71× KDP	129.63	51,52
4M5B2SC		Monoclinic $P\text{c}$	4.2 × urea	141	S5
DMMC		Monoclinic $P2_1$	58 × KDP	95.59	S6
3,4-DABP		Monoclinic C_2	2.3 × KDP	121	S7
BBP		Orthorhombic $P2_12_12_1$	2.03 × KDP	280	S8
TTMP		Orthorhombic $P\text{na}2_1$	1.95 × urea	152.65	S9
5B2SNC		Monoclinic $C\text{c}$	26 × urea	166.4	S10
HPMP		Orthorhombic $P\text{ca}2_1$	1.86 × KDP	95	S11
PMC		Orthorhombic $P2_12_12_1$	6 × urea	341	S12
MNC		Orthorhombic $P2_12_12_1$	55 × urea	-	S13
5CT4MP		Monoclinic $P\text{c}$	1.6 × urea	115	S14
3-CPDP		Triclinic $P1$	1.4 × urea	154	S15
4BC		-	1.14 × urea	-	S16

Crystal Name	Chemical Structure	Space Group	SHG *	Melting point	Ref.
2MPNP		Orthorhombic $P\text{ca}2_1$	2.75 × KDP	142.53	S17
2,4,5-TMBC		Orthorhombic $P2_12_12_1$	1.8 × urea	-	S18
BPP		Monoclinic $P2_1$	1.4 × urea		S19
CPP		Monoclinic $P2_1$	3.67 × urea	-	S20
MPP		Orthorhombic $P\text{na}2_1$	4.7 × urea	81	S21
DCPP		Monoclinic $P2_1$	≈ urea	146.9	S22
MMPP		Orthorhombic $P\text{na}2_1$	3.15 × urea	80	S23
MLS		Orthorhombic $P\text{na}2_1$	1.5 × OH1 at 2090 nm	166	31
OH-IPO		Orthorhombic $F\text{dd}2$	0.7 × OH1 at 2090 nm	210	33
UOH1		Tetragonal $I4_1$	3.3 × urea at 800nm	172	30
NPP		Monoclinic $P2_1$	d_{21}=48 pm/V at 1150 nm	116	42
BNA		Orthorhombic $P\text{na}2_1$	d_{33}=234 pm/V at 1064 nm	106	43
MPMOI		Orthorhombic $P2_12_12_1$	3.7 × KDP	175	This work

*The powder second harmonic generation test was performed under 1064 nm fundamental wavelength.

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