

Supplementary Information

Bulk crystal growth and characterization of semi-organic nonlinear optical crystal tri-diethylammonium hexachlorobismuthate (TDCB)

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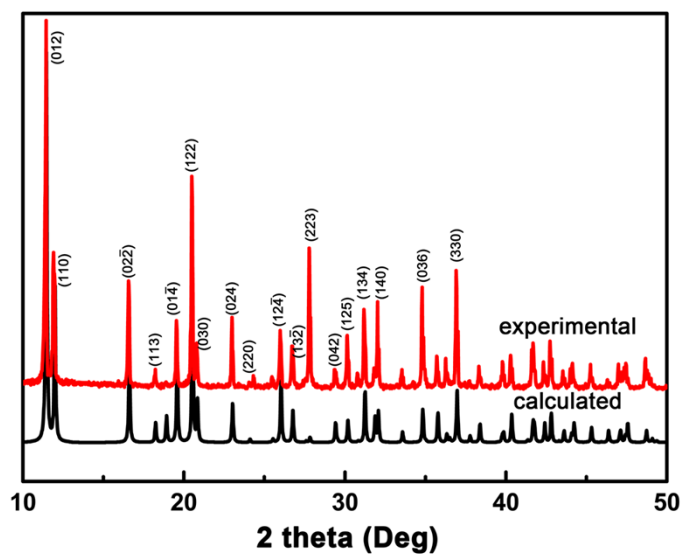


Figure S1. Simulated and experimental XRD powder patterns for TDCB.

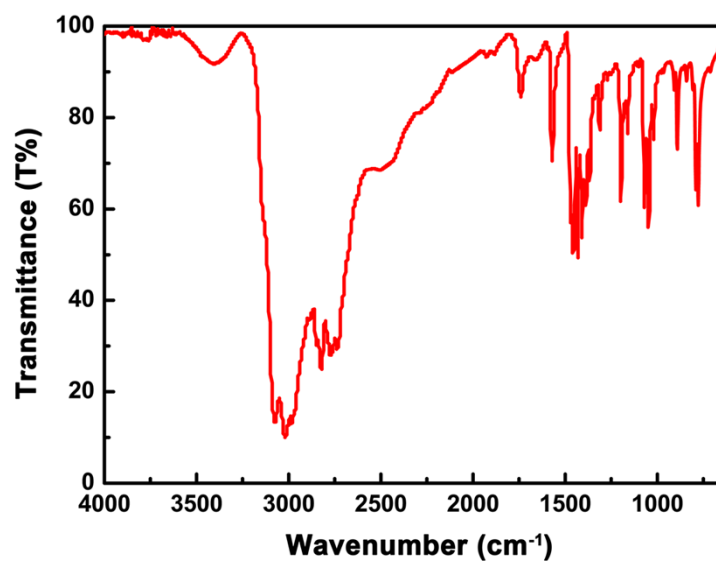


Figure S2. The FT-IR spectrum of TDCB.

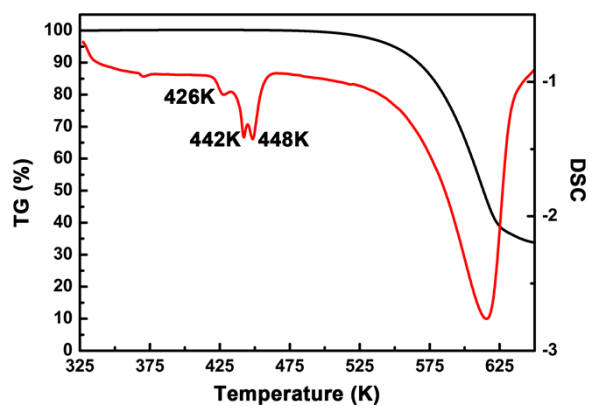


Figure S3. Thermogravimetric analysis for TDCB.

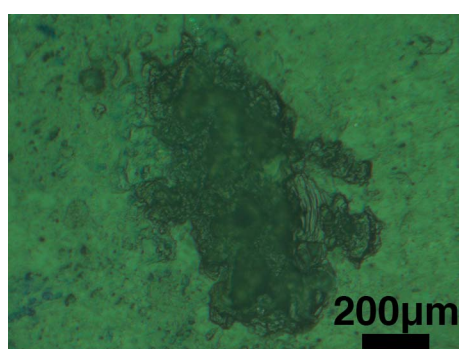


Figure S4. Micrograph of the laser-induced damage pattern.

Table S1. Crystal data and structure refinement for TDCB.

Empirical formula	$C_{12} H_{36} N_3 Bi Cl_6$
Formula weight	644.12
Temperature/K	100
Crystal system	trigonal
Space group	R3c
a (Å)	14.699 (4)
b (Å)	14.699 (4)
c (Å)	19.102 (5)
α (deg)	90
β (deg)	90
γ (deg)	120
V (Å ³)	3574.2 (17)
ρ_{calcd} (g/cm ³)	1.795
λ (Mo K α) (Å)	0.71073
Collected reflns	12907
Unique reflns	1816
Parameters	70

R (int)	0.0261
$R_1 [I > 2\sigma(I)]$	0.0109
$wR_2 [I > 2\sigma(I)]$	0.0295
GOF	1.092