

Electronic Supplementary Information (ESI) for:

**Effect of polarizable lone pair cations on the second-harmonic generation (SHG) properties of noncentrosymmetric (NCS)  $\text{Bi}_{2-x}\text{Y}_x\text{TeO}_5$  ( $x = 0-0.2$ )**

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Table S1. Atomic Coordinates, Displacement Parameters, and Occupancies for  $\text{Bi}_2\text{TeO}_5$

Table S2. Atomic Coordinates, Displacement Parameters, and Occupancies for  $\text{Bi}_{1.9}\text{Y}_{0.1}\text{TeO}_5$

Table S3. Atomic Coordinates, Displacement Parameters, and Occupancies for  $\text{Bi}_{1.8}\text{Y}_{0.2}\text{TeO}_5$

Figure S1. Infrared spectra of  $\text{Bi}_{2-x}\text{Y}_x\text{TeO}_5$  ( $x = 0, 0.1, \text{ and } 0.2$ )

Figure S2. Phase matching, i.e., particle size vs. SHG intensity data for  $\text{Bi}_2\text{TeO}_5$ . The curve is drawn to guide the eye and is not a fit to the data.

Figure S3. Phase matching, i.e., particle size vs. SHG intensity data for  $\text{Bi}_{1.9}\text{Y}_{0.1}\text{TeO}_5$ . The curve is drawn to guide the eye and is not a fit to the data.

Figure S4. Phase matching, i.e., particle size vs. SHG intensity data for  $\text{Bi}_{1.8}\text{Y}_{0.2}\text{TeO}_5$ . The curve is drawn to guide the eye and is not a fit to the data.

Figure S5. EDAX spectra for  $\text{Bi}_{2-x}\text{Y}_x\text{TeO}_5$  ( $x = 0, 0.1, \text{ and } 0.2$ )

Table S1. Atomic Coordinates, Displacement Parameters, and Occupancies for Bi<sub>2</sub>TeO<sub>5</sub>

<i>Atom</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>U<sub>iso</sub></i>	<i>Occupancy</i>
Bi(1)	0.39169(7)	0.08574(11)	0.4848(6)	0.0073(3)	1.0
Bi(2)	0.87472(16)	0.25	0.0009(3)	0.0068(4)	1.0
Bi(3)	0.62249(18)	0.25	0.52333(19)	0.0040(3)	1.0
Te(1)	0.13291(14)	0.08008(14)	-0.0154(3)	0.0059(4)	1.0
O(1)	0.26339(19)	0.04448(14)	0.1439(3)	0.0209(4)	1.0
O(2)	0.5	0	0.7942(3)	0.0110(4)	1.0
O(3)	0.06710(19)	0.14761(15)	0.2224(3)	0.0198(4)	1.0
O(4)	0.7081(3)	0.25	0.8703(3)	0.0170(4)	1.0
O(5)	0.47924(16)	0.16057(14)	0.2041(3)	0.0109(4)	1.0
O(6)	0.20457(15)	0.15767(14)	0.7881(3)	0.0161(4)	1.0

Table S2. Atomic Coordinates, Displacement Parameters, and Occupancies for Bi<sub>1.9</sub>Y<sub>0.1</sub>TeO<sub>5</sub>

<i>Atom</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>U<sub>iso</sub></i>	<i>Occupancy</i>
Bi(1)/Y(1)	0.39170(10)	0.08556(16)	0.4844(5)	0.0073(3)	0.95/0.05
Bi(2)/Y(2)	0.8740(3)	0.25	0.0009(7)	0.0165(3)	0.95/0.05
Bi(3)/Y(3)	0.6222(3)	0.25	0.5222(5)	0.0118(4)	0.95/0.05
Te(1)	0.13287(19)	0.0805(2)	-0.0187(7)	0.0055(4)	1.0
O(1)	0.2652(3)	0.0442(2)	0.1443(8)	0.0290(4)	1.0
O(2)	0.5	0	0.7901(7)	0.0095(3)	1.0
O(3)	0.0681(3)	0.1475(3)	0.2223(8)	0.0270(4)	1.0
O(4)	0.7076(5)	0.25	0.8688(8)	0.0201(4)	1.0
O(5)	0.4795(2)	0.16027(19)	0.2016(5)	0.0093(4)	1.0
O(6)	0.2057(3)	0.1580(3)	0.7835(7)	0.0268(4)	1.0

Table S3. Atomic Coordinates, Displacement Parameters, and Occupancies for  $\text{Bi}_{1.8}\text{Y}_{0.2}\text{TeO}_5$

<i>Atom</i>	<i>x</i>	<i>y</i>	<i>z</i>	$U_{iso}$	<i>Occupancy</i>
Bi(1)/Y(1)	0.39129(11)	0.08551(19)	0.4849(6)	0.0081(3)	0.90/0.10
Bi(2)/Y(2)	0.8740(3)	0.25	0.0013(9)	0.0251(3)	0.90/0.10
Bi(3)/Y(3)	0.6212(3)	0.25	0.5229(6)	0.0170(3)	0.90/0.10
Te(1)	0.1328(2)	0.0805(2)	-0.0171(8)	0.0059(3)	1.0
O(1)	0.2663(4)	0.0439(3)	0.1423(10)	0.0405(4)	1.0
O(2)	0.5	0	0.7882(8)	0.0089(3)	1.0
O(3)	0.0680(3)	0.1478(3)	0.2237(10)	0.0363(3)	1.0
O(4)	0.7079(6)	0.25	0.8699(10)	0.0266(3)	1.0
O(5)	0.4801(3)	0.1604(2)	0.2012(6)	0.0102(4)	1.0
O(6)	0.2062(3)	0.1580(3)	0.7807(9)	0.0322(3)	1.0

Figure S1. Infrared spectra of  $\text{Bi}_{2-x}\text{Y}_x\text{TeO}_5$  ( $x = 0, 0.1, \text{ and } 0.2$ )

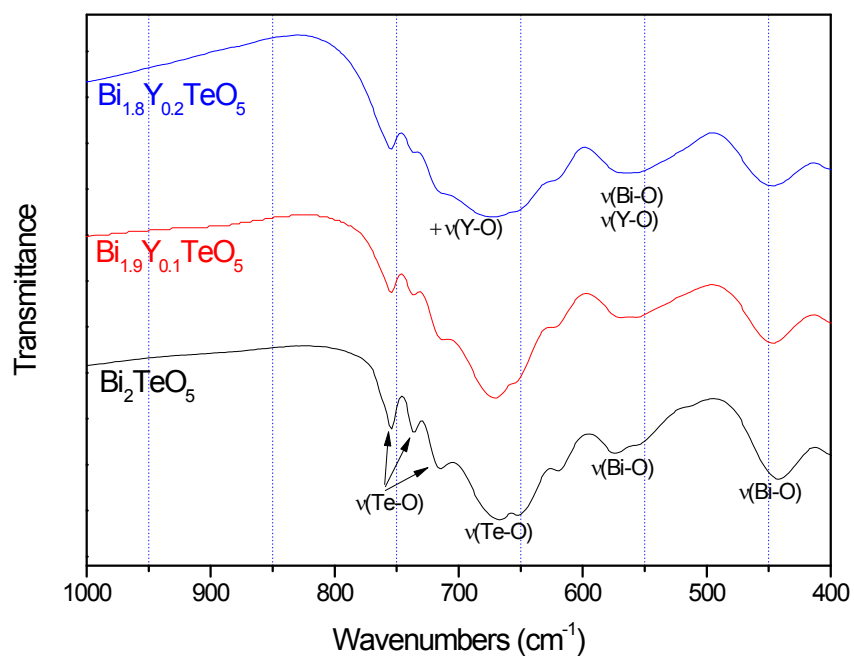


Figure S2. Phase matching, i.e., particle size vs. SHG intensity data for  $\text{Bi}_2\text{TeO}_5$ . The curve is drawn to guide the eye and is not a fit to the data.

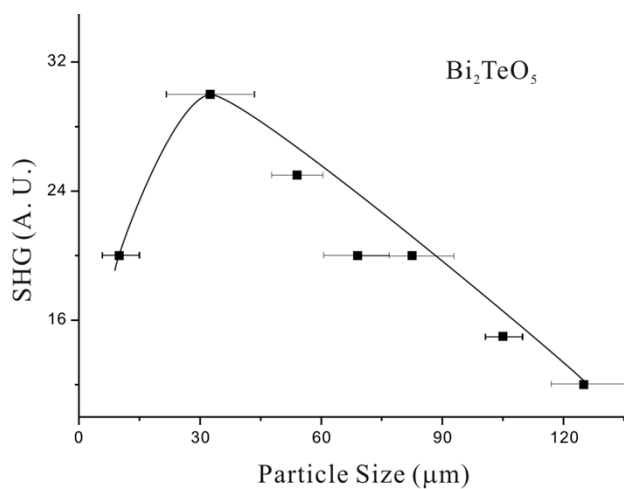


Figure S3. Phase matching, i.e., particle size vs. SHG intensity data for  $\text{Bi}_{1.9}\text{Y}_{0.1}\text{TeO}_5$ . The curve is drawn to guide the eye and is not a fit to the data.

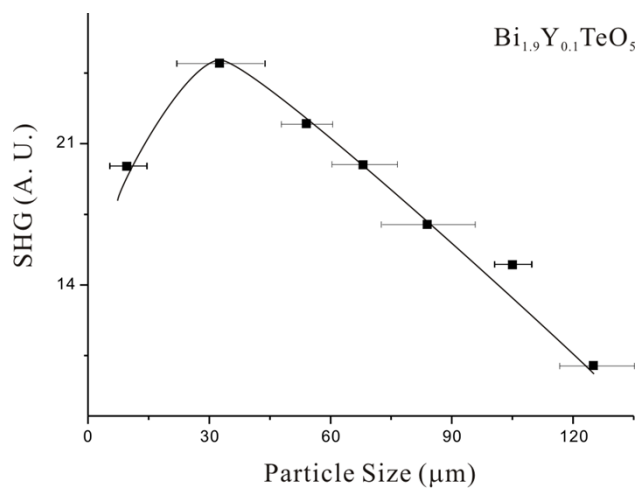


Figure S4. Phase matching, i.e., particle size vs. SHG intensity data for  $\text{Bi}_{1.8}\text{Y}_{0.2}\text{TeO}_5$ . The curve is drawn to guide the eye and is not a fit to the data.

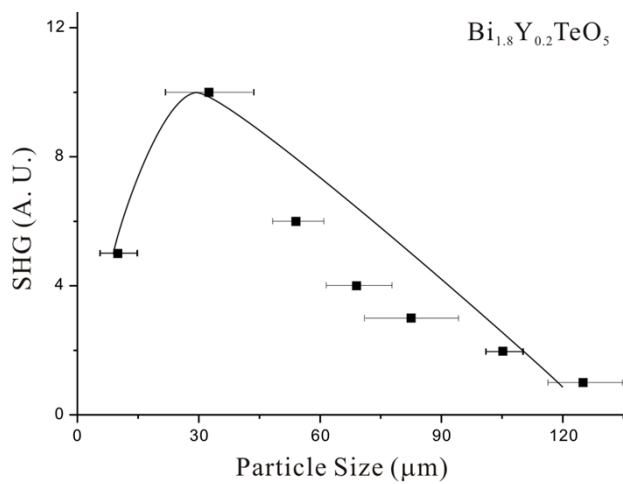


Figure S5. EDAX spectra for  $\text{Bi}_{2-x}\text{Y}_x\text{TeO}_5$  ( $x = 0, 0.1, \text{ and } 0.2$ )

