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Supporting information for article:

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Second harmonic generation from the “centrosymmetric” crystals

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Supporting information

The crystal data were refined purposely in the space group *Cc* to show the presence of both non-centrosymmetric and centrosymmetric packing in the crystal. The crystal was originally refined in the space group *C2/c* before (Medishetty, 2014, CCDC No. 979138).

Table S1 Cell data for **1** at different temperatures

	1 (E219)	1 (E210)
<i>Temperature (K)</i>	170(2)	295(2)
<i>Sp. Grp</i>	<i>Cc</i>	<i>Cc</i>
<i>a</i> (Å)	24.746(2)	24.843(2)
<i>b</i> (Å)	12.212(1)	12.245(1)
<i>c</i> (Å)	15.653(1)	15.720(1)
<i>β</i> (deg)	109.192(1)	109.498(2)
<i>V</i> (Å ³)	4467.2(6)	4507.9(7)
<i>Z</i>	4	4
<i>D</i> _{calc} (g/cm ³)	1.454	1.440
<i>μ</i> (mm ⁻¹)	1.134	1.124
GOF	1.046	1.010
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0323	0.0371
<i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0845	0.0898

Only selected data are shown here since they are very similar and no trend has been found. Other data can be retrieved: CCDC 1031432-1031436

Table S2 The Flack parameters for **1** obtained for two single crystals at different temperatures.

Temperature	SHG found	Flack parameter for the Crystal showing High SHG	Flack parameter for the Crystal showing Low SHG
170 K	low	0.34(3)	0.38(3)
295 K	Medium	0.10(3)	0.41(3)
80 K	high	-	0.37(3)

The Flack and Hooft parameters were also obtained using OLEX2 but the parameters changed and no correlation was found.

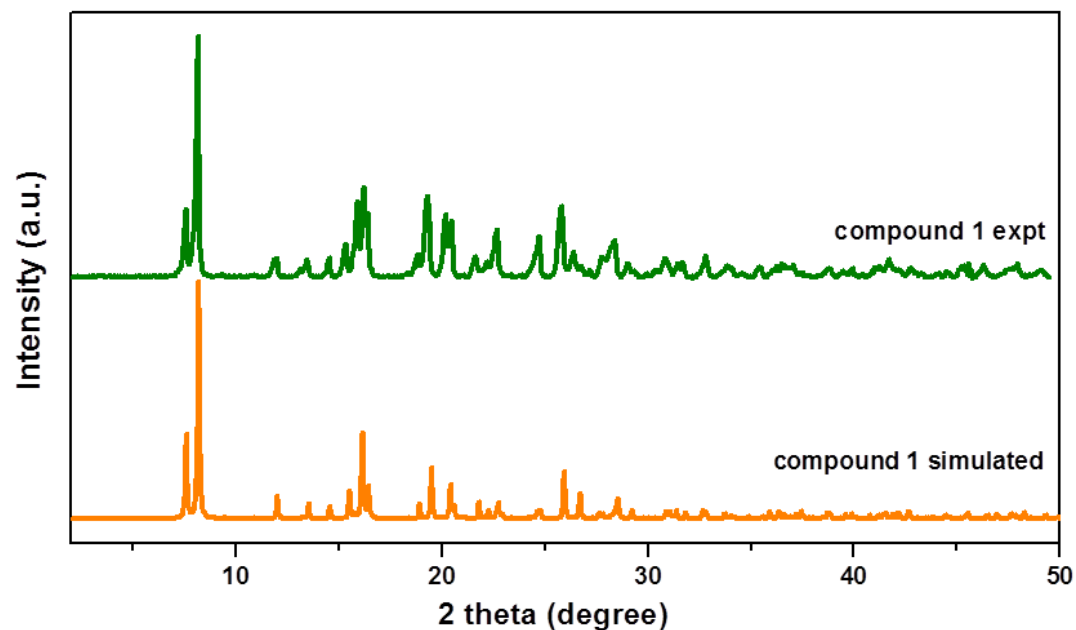


Figure S1 PXRD pattern of **1**.

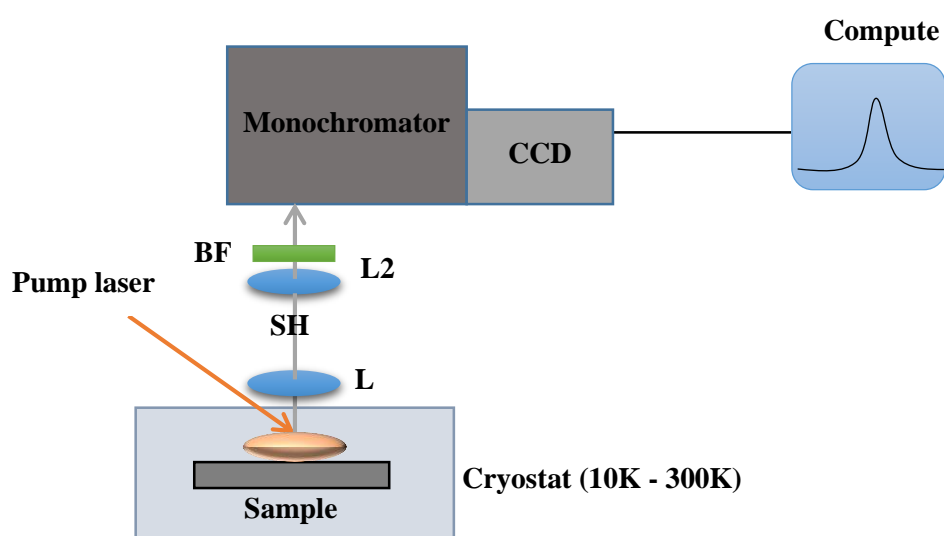


Figure S2 Schematic view of SHG measurements.



Figure S3 Experimental microscope set up for SHG measurement at room temperature.

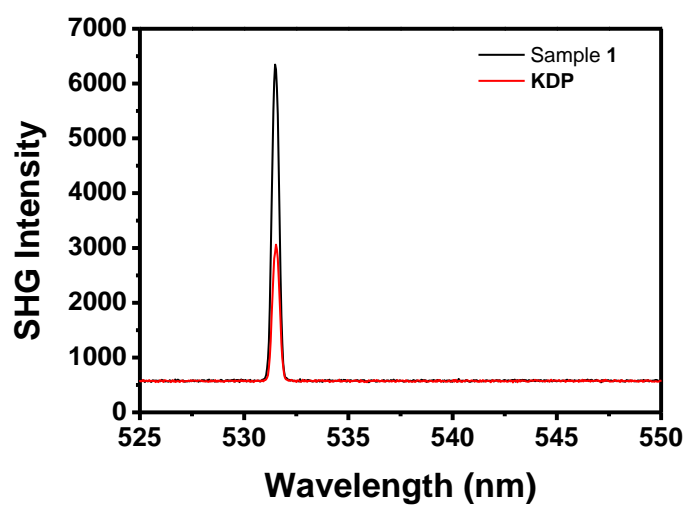


Figure S4 SHG measurement of KDP and 1.

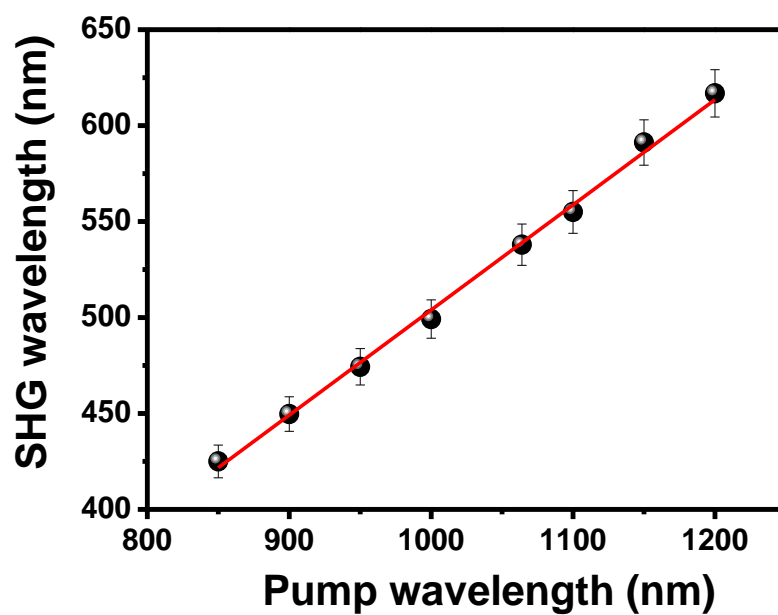


Figure S5 Excitation wavelength dependent SHG wavelength measurement of **1**.

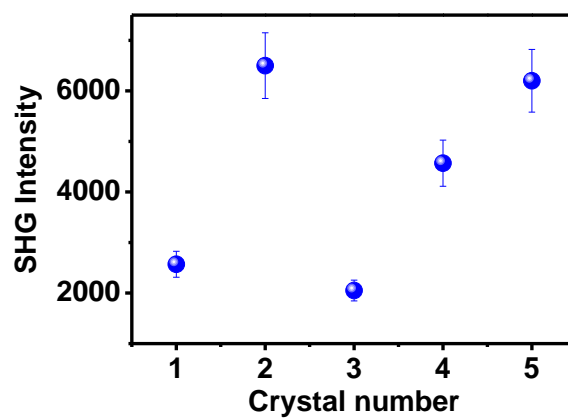


Figure S6 SHG intensities of different crystals from the same batch of **1**.