

Supporting Information

Effect of Co-substitution of Heterovalent Ions Ga³⁺ and Sb⁵⁺ on Nonlinear Optical Effects in Phosphate Crystals

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Figure S1. High-resolution X-ray photoelectron spectra for O1s core level of KTP.

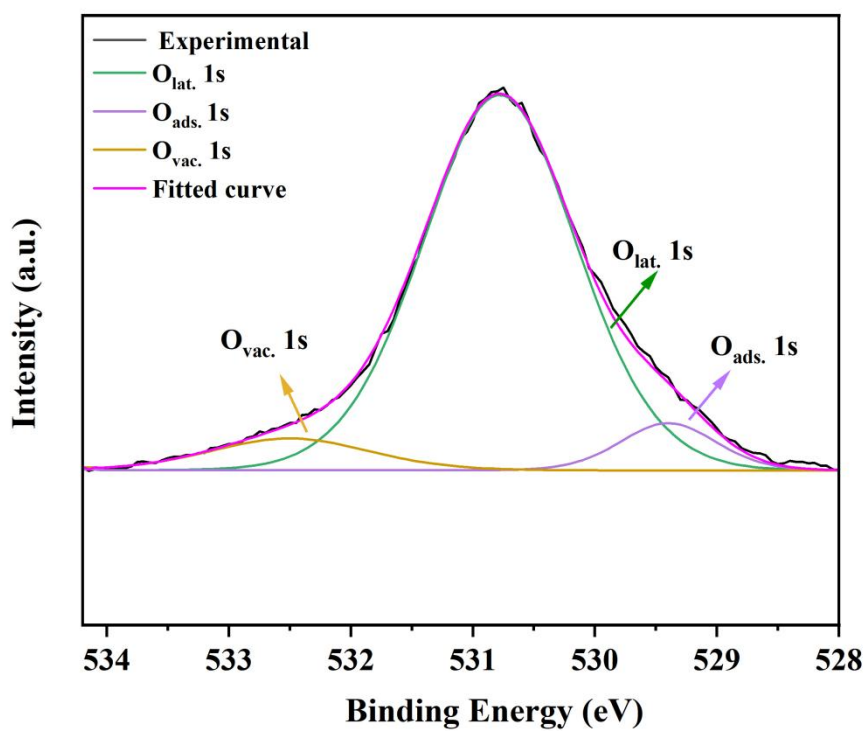


Table S1. Dipole moment calculations for Ga³⁺:Sb⁵⁺:KTP and KTP.

Species	Dipole Moment				Magnitude
	x(a)	y(b)	z(c)	Debye	$\times 10^{-4}$ esu·cm/Å ³
Ga ³⁺ :Sb ⁵⁺ :KTP					
Ga-TiO ₆ Ti ₁₉	-2.611	1.381	2.497	3.867	0.002
Ga-TiO ₆ Ti ₃₅	2.611	1.381	2.497	3.867	0.002
Sb-TiO ₆ Ti ₄	5.161	2.977	3.345	6.832	0.004
Sb-TiO ₆ Ti ₁₁₆	-5.161	2.977	3.345	6.832	0.004
Ga-PO ₄ P ₃₇	0.226	0.026	0.577	0.620	0.000
Ga-PO ₄ P ₃₈	0.551	0.174	0.258	0.633	0.000
Ga-PO ₄ P ₅₃	0.226	0.026	0.577	0.620	0.000
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SbO ₆	-1.32	0.05	0.54	1.43	0.000
GaO ₆	0.30	-0.83	0.38	0.97	0.000
Pure KTP					
TiO ₆ Ti ₈	0.886	-0.468	0.847	1.312	0.001
TiO ₆ Ti ₁₂	1.751	1.010	1.135	2.318	0.001
PO ₄ P ₁₆	-0.321	-0.036	0.819	0.881	0.001
PO ₄ P ₂₀	0.783	-0.246	0.367	0.899	0.001