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SUPPLEMENTARY INFORMATION

$Ba_5CdGa_6Se_{15}$, a congruently-melting infrared nonlinear optical material with strong SHG response

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Table S1. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $Ba_5CdGa_6Se_{15}$.

Table S2. Interatomic distances (Å) for $Ba_5CdGa_6Se_{15}$.

Figure S1. Powder XRD pattern of $Ba_5CdGa_6Se_{15}$. The inset shows an SEM image of a typical crystal of this compound.

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Table S1 Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for $Ba_5CdGa_6Se_{15}$

Atom	Wyckoff position	Occupancy	*x*	*y*	*z*	U_{eq} (Å^2) [a]
Ba1	8*c*	1	0.11158(2)	0.16313(3)	0.53149(8)	0.02311(13)
Ba2	8*c*	1	0.61573(2)	0.13084(3)	0.49176(8)	0.01937(11)
Ba3	4*b*	1	¼	0.15388(4)	0.08079(11)	0.01982(15)
*M*1	8*c*	1 Ga	0.02912(4)	0.19363(5)	0.06038(14)	0.01622(19)
*M*2	8*c*	0.408(9) Cd, 0.592(9) Ga	0.15858(4)	0.47028(4)	0.47523(14)	0.0230(3)
*M*3	4*b*	1 Ga	¼	0.30720(7)	0.6096(2)	0.0174(3)
*M*4	4*b*	0.195(12) Cd, 0.805(12) Ga	¼	0.47167(7)	0.95279(19)	0.0181(4)
*M*5	4*a*	1 Ga	0	0	0.0000(2)	0.0172(3)
Se1	8*c*	1	0.00009(4)	0.09428(4)	0.24606(15)	0.01900(18)
Se2	8*c*	1	0.01066(4)	0.30348(5)	0.22983(15)	0.02121(19)
Se3	8*c*	1	0.07855(5)	0.50724(5)	0.27451(16)	0.0296(2)
Se4	8*c*	1	0.12625(3)	0.19928(4)	0.01776(14)	0.01841(18)
Se5	8*c*	1	0.15950(4)	0.34053(5)	0.48910(15)	0.02062(18)
Se6	8*c*	1	0.16694(4)	0.02270(5)	0.31479(15)	0.0231(2)
Se7	4*b*	1	¼	0.18387(6)	0.57922(19)	0.0178(2)
Se8	4*b*	1	¼	0.50882(7)	0.3097(2)	0.0257(3)
Se9	4*b*	1	¼	0.84371(7)	0.46676(19)	0.0184(2)

[a] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S2 Interatomic distances (Å) for $Ba_5CdGa_6Se_{15}$

Ba1–Se2	3.3042(12)	Ba3–Se7	3.3701(15)
Ba1–Se4	3.3123(11)	Ba3–Se6 (×2)	3.5737(12)
Ba1–Se6	3.3314(11)	Ba3–Se9	3.7143(15)
Ba1–Se7	3.3942(6)	Ga1–Se1	2.3728(13)
Ba1–Se3	3.4856(11)	Ga1–Se4	2.3742(13)
Ba1–Se4	3.4893(11)	Ga1–Se2	2.3923(13)
Ba1–Se1	3.5523(11)	Ga1–Se2	2.4265(13)
Ba1–Se5	3.6027(11)	Cd/Ga2–Se3	2.4561(15)
Ba2–Se2	3.2492(11)	Cd/Ga2–Se6	2.4706(14)
Ba2–Se4	3.2691(10)	Cd/Ga2–Se5	2.4876(12)
Ba2–Se9	3.2959(5)	Cd/Ga2–Se8	2.5805(11)
Ba2–Se1	3.3200(11)	Ga3–Se7	2.3713(18)
Ba2–Se3	3.3638(11)	Ga3–Se5 (×2)	2.4205(11)
Ba2–Se6	3.4011(11)	Ga3–Se9	2.4660(19)
Ba2–Se5	3.5028(11)	Cd/Ga4–Se6 (×2)	2.4177(12)
Ba2–Se5	3.5359(11)	Cd/Ga4–Se9	2.4532(18)
Ba3–Se4 (×2)	3.1517(9)	Cd/Ga4–Se8	2.4679(19)
Ba3–Se8	3.3083(16)	Ga5–Se3 (×2)	2.4239(13)
Ba3–Se7	3.3496(15)	Ga5–Se1 (×2)	2.4323(13)

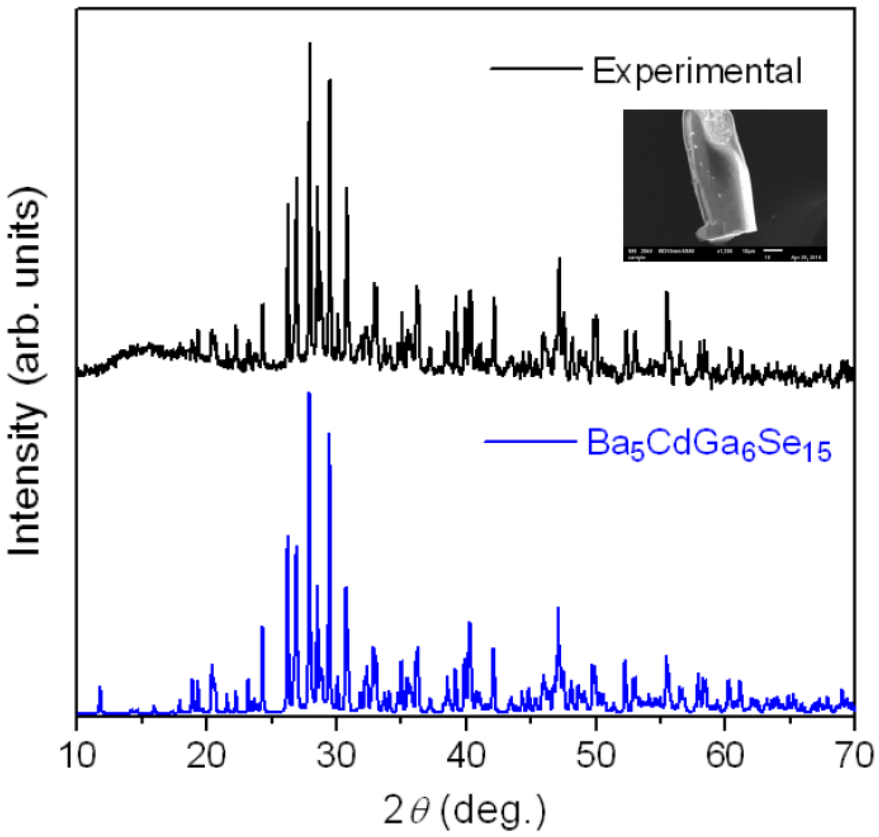

Figure S1. Powder XRD pattern of $Ba_5CdGa_6Se_{15}$. The inset shows an SEM image of a typical crystal of this compound.