Supporting Information

$Na_2Cd_7B8O_{20}$: A New Noncentrosymmetric Compound with Special $[B_3O_7]$ Units

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Figure S1. The XRD patterns for $Na_2Cd_7B_8O_{20}$. The black curve is the calculated one, the red curve is the pattern of the stoichiometric powder mixtures, the blue curve is the pattern of powder mixture with excessive Na and the green curve is the pattern of powder mixture with excessive Cd.

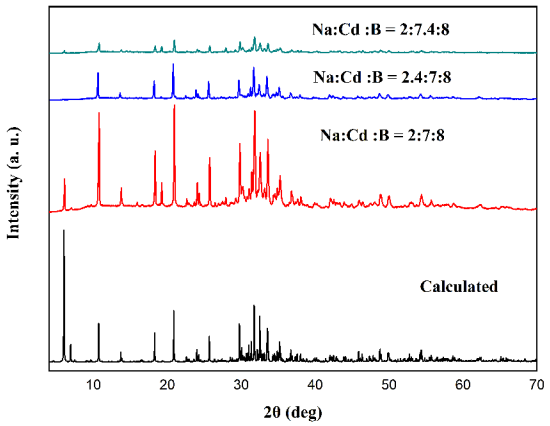

Figure S2. The structure of the two-dimensional layer composed of CdO_n (n = 6, 7) polyhedra shown in blue and Na/CdO_n (n = 5, 6) polyhedra in green extending in the (010) plane.

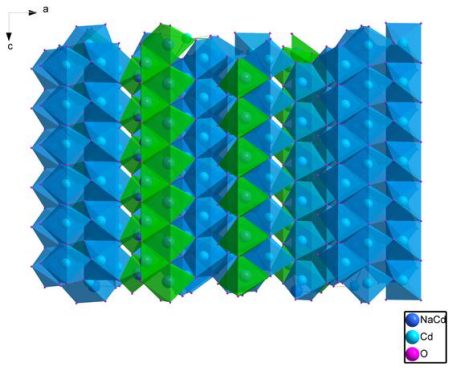

Figure S3. The structure of $[B_3O_7]$ unit.

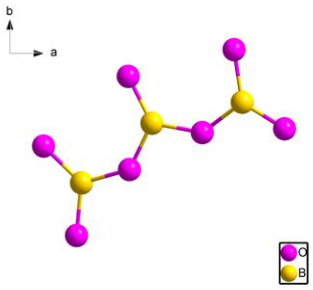

Figure S4. The IR spectrum of $Na_2Cd_7B_8O_{20}$.

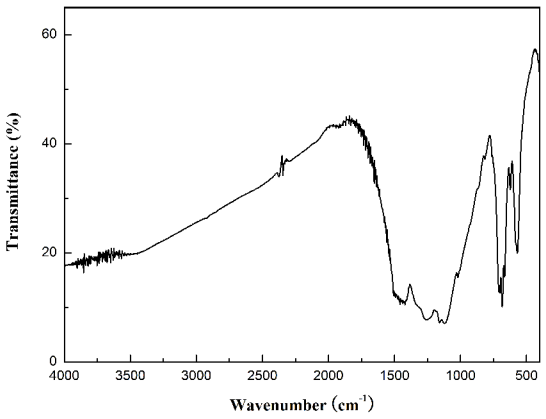

Figure S5. SHG measurements of $Na_2Cd_7B_8O_{20}$.

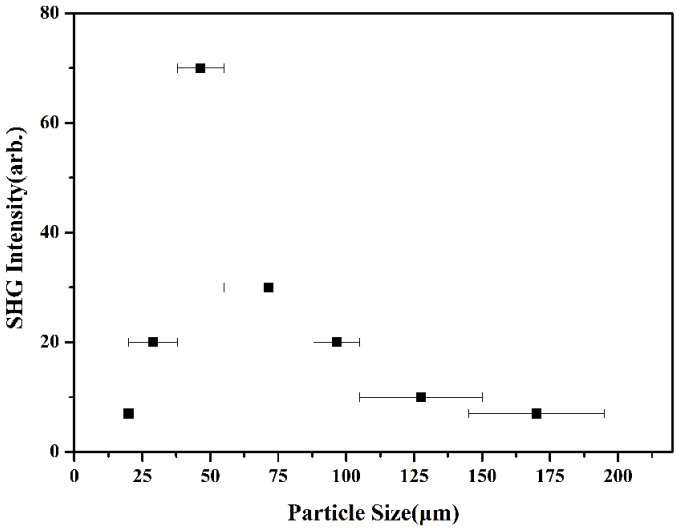

Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Na_2Cd_7B_8O_{20}$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	*x/a*	*y/b*	*z/c*	*Ueq*	occ
Na(1)/Cd(1)	1995(1)	1433(1)	-3227(1)	13(1)	0.276/0.724
Na(2)/Cd(2)	1509(1)	1788(1)	-1220(2)	7(1)	0.456/0.544
Na(3)/Cd(3)	2734(1)	247(1)	9857(4)	7(1)	0.393/0.607
Na(4)/Cd(4)	1879(1)	2187(1)	3573(4)	7(1)	0.375/0.625
Cd(5)	1798(1)	918(1)	954(3)	17(1)	1
Cd(6)	1202(1)	1004(1)	-2734(3)	14(1)	1
Cd(7)	709(1)	590(1)	1654(3)	12(1)	1
Cd(8)	1081(1)	171(1)	6554(3)	16(1)	1
Cd(9)	924(1)	1493(1)	-7660(3)	12(1)	1
Cd(10)	124(1)	934(1)	944(3)	12(1)	1
Cd(11)	323(1)	1433(1)	-3712(3)	20(1)	1
Cd(12)	2349(1)	630(1)	5194(3)	12(1)	1
Na(5)	0	0	3300(80)	123(7)	1
Na(6)	3326(3)	68(3)	4540(70)	142(6)	1
B(1)	495(3)	151(2)	6880(50)	13(3)	1
B(2)	1283(3)	2215(2)	4690(50)	10(3)	1
B(3)	1341(3)	553(2)	2610(40)	10(3)	1
B(4)	2984(3)	635(2)	13770(50)	12(3)	1
B(5)	1777(3)	457(2)	5890(50)	11(3)	1
B(6)	1509(3)	1328(2)	-6060(50)	11(3)	1
B(7)	3433(3)	544(2)	10300(40)	8(3)	1
B(8)	2126(3)	200(3)	9160(50)	14(3)	1
B(9)	2218(3)	1870(2)	-930(50)	9(3)	1
B(10)	662(3)	1049(2)	-3530(50)	10(3)	1
B(11)	2335(3)	1093(2)	1940(50)	9(3)	1
B(12)	148(3)	431(2)	-1380(50)	12(3)	1
O(1)	2311(2)	360(2)	9840(30)	10(2)	1

O(2)	806(2)	849(2)	-3480(30)	16(2)	1
O(3)	2774(2)	520(2)	14730(30)	15(2)	1
O(4)	786(2)	1251(2)	-2730(30)	15(2)	1
O(5)	1897(2)	660(2)	5760(30)	14(2)	1
O(6)	1471(2)	2055(2)	3990(30)	17(2)	1
O(7)	685(2)	319(2)	6720(30)	14(2)	1
O(8)	1120(2)	443(2)	1620(30)	12(2)	1
O(9)	1963(2)	1918(2)	-1440(30)	18(2)	1
O(10)	1267(2)	1280(2)	-7580(30)	16(2)	1
O(11)	1193(2)	-57(2)	11450(30)	17(2)	1
O(12)	1384(2)	775(1)	1750(30)	11(2)	1
O(13)	2378(2)	877(2)	330(30)	27(3)	1
O(14)	1628(2)	1538(2)	3520(30)	18(2)	1
O(15)	2851(2)	24(2)	4970(30)	20(2)	1
O(16)	2103(2)	1194(2)	1740(30)	20(2)	1
O(17)	1888(2)	263(2)	7360(30)	16(2)	1
O(18)	3182(2)	503(2)	11790(40)	19(2)	1
O(19)	401(2)	1046(2)	-4190(30)	15(2)	1
O(20)	525(2)	1637(2)	-8290(30)	17(2)	1
O(21)	278(2)	587(2)	590(30)	19(2)	1
O(22)	1634(2)	1160(2)	-4000(30)	14(2)	1
O(23)	1953(2)	2429(2)	-1410(30)	21(2)	1
O(24)	1044(2)	2157(2)	6480(30)	17(2)	1
O(25)	2321(2)	1660(2)	-1570(30)	15(2)	1
O(26)	2375(2)	2056(2)	300(40)	27(3)	1
O(27)	1050(2)	1753(2)	-12310(30)	13(2)	1
O(28)	1527(2)	419(2)	4470(30)	18(2)	1
O(29)	239(2)	210(2)	7790(30)	16(2)	1
O(30)	45(2)	1301(2)	1190(30)	15(2)	1

Table S2. Selected bond distances (Å) and angles (deg) for $Na_2Cd_7B_8O_{20}$.

Cd(1)-O(25)	2.217(9)	Cd(12)-O(5)	2.344(9)
Cd(1)-O(16)	2.259(11)	Cd(12)-O(1)#1	2.413(10)
Cd(1)-O(14)#1	2.269(9)	Na(1)-O(25)	2.217(9)
Cd(1)-O(16)#1	2.275(11)	Na(1)-O(16)	2.259(11)
Cd(1)-O(22)	2.469(9)	Na(1)-O(14)#1	2.269(9)
Cd(2)-O(14)	2.258(10)	Na(1)-O(16)#1	2.275(11)
Cd(2)-O(6)#1	2.263(10)	Na(1)-O(22)	2.469(9)
Cd(2)-O(6)	2.368(11)	Na(2)-O(14)	2.258(10)
Cd(2)-O(14)#1	2.386(11)	Na(2)-O(6)#1	2.263(10)
Cd(2)-O(27)#2	2.403(9)	Na(2)-O(6)	2.368(11)
Cd(2)-O(9)	2.463(9)	Na(2)-O(14)#1	2.386(11)
Cd(3)-O(15)	2.193(10)	Na(2)-O(27)#2	2.403(9)
Cd(3)-O(15)#2	2.250(10)	Na(2)-O(9)	2.463(9)
Cd(3)-O(1)	2.276(8)	Na(3)-O(15)	2.193(10)
Cd(3)-O(3)	2.307(10)	Na(3)-O(15)#2	2.250(10)
Cd(3)-O(3)#1	2.370(10)	Na(3)-O(1)	2.276(8)
Cd(3)-O(18)	2.836(10)	Na(3)-O(3)	2.307(10)
Cd(4)-O(23)	2.233(11)	Na(3)-O(3)#1	2.370(10)
Cd(4)-O(23)#2	2.243(10)	Na(3)-O(18)	2.836(10)
Cd(4)-O(6)	2.248(9)	Na(4)-O(23)	2.233(11)
Cd(4)-O(9)#2	2.351(10)	Na(4)-O(23)#2	2.243(10)
Cd(4)-O(9)	2.358(11)	Na(4)-O(6)	2.248(9)
Cd(5)-O(16)	2.273(9)	Na(4)-O(9)#2	2.351(10)
Cd(5)-O(5)	2.280(10)	Na(4)-O(9)	2.358(11)
Cd(5)-O(12)	2.310(9)	Na(5)-O(29)	2.31(2)
Cd(5)-O(22)	2.350(9)	Na(5)-O(29)#5	2.31(2)
Cd(5)-O(5)#1	2.374(10)	Na(5)-O(29)#6	2.55(2)
Cd(5)-O(22)#2	2.375(10)	Na(5)-O(29)#1	2.55(2)
Cd(6)-O(12)	2.234(9)	Na(6)-O(17)#9	2.35(2)
Cd(6)-O(2)	2.251(9)	Na(6)-O(15)	2.46(2)

Cd(6)-O(10)	2.329(11)	Na(6)-O(24)#10	2.48(2)
Cd(6)-O(10)#2	2.401(10)	Na(6)-O(11)#9	2.56(2)
Cd(6)-O(22)	2.444(9)	Na(6)-O(24)#11	2.72(2)
Cd(6)-O(12)#1	2.482(9)	Na(6)-O(18)#1	2.82(2)
Cd(6)-O(4)	2.587(10)	B(1)-O(23)#8	1.357(17)
Cd(7)-O(21)	2.254(10)	B(1)-O(7)	1.392(17)
Cd(7)-O(8)	2.286(9)	B(1)-O(29)	1.398(16)
Cd(7)-O(2)#2	2.293(10)	B(2)-O(11)#4	1.367(17)
Cd(7)-O(7)#1	2.310(10)	B(2)-O(6)	1.369(17)
Cd(7)-O(7)	2.342(10)	B(2)-O(24)	1.413(17)
Cd(7)-O(2)	2.360(10)	B(3)-O(12)	1.353(16)
Cd(8)-O(11)	2.205(10)	B(3)-O(8)	1.354(16)
Cd(8)-O(7)	2.219(8)	B(3)-O(28)	1.390(17)
Cd(8)-O(11)#1	2.260(10)	B(4)-O(3)	1.318(17)
Cd(8)-O(8)	2.317(10)	B(4)-O(20)#13	1.362(17)
Cd(8)-O(8)#2	2.349(10)	B(4)-O(18)	1.445(17)
Cd(8)-O(28)	2.812(5)	B(5)-O(5)	1.345(17)
Cd(9)-O(10)	2.167(9)	B(5)-O(17)	1.365(16)
Cd(9)-O(20)	2.235(9)	B(5)-O(28)	1.393(17)
Cd(9)-O(27)	2.288(9)	B(6)-O(22)	1.372(17)
Cd(9)-O(4)	2.302(9)	B(6)-O(10)	1.377(17)
Cd(9)-O(4)#1	2.335(10)	B(6)-O(14)#1	1.383(17)
Cd(9)-O(27)#2	2.454(9)	B(7)-O(27)#13	1.339(16)
Cd(10)-O(21)	2.183(10)	B(7)-O(24)#10	1.384(16)
Cd(10)-O(30)	2.195(9)	B(7)-O(18)	1.405(16)
Cd(10)-O(19)#2	2.275(9)	B(8)-O(15)#3	1.346(17)
Cd(10)-O(19)	2.342(10)	B(8)-O(1)	1.357(17)
Cd(10)-O(25)#7	2.365(10)	B(8)-O(17)	1.422(17)
Cd(10)-O(25)#12	2.371(10)	B(9)-O(9)	1.352(16)
Cd(11)-O(20)	2.218(10)	B(9)-O(25)	1.362(16)
Cd(11)-O(19)	2.313(9)	B(9)-O(26)	1.418(16)
Cd(11)-O(30)	2.325(10)	B(10)-O(19)	1.365(17)

Cd(11)-O(30)#1	2.371(10)	B(10)-O(4)	1.372(16)
Cd(11)-O(20)#2	2.423(11)	B(10)-O(2)	1.391(16)
Cd(11)-O(13)#12	2.606(12)	B(11)-O(16)	1.336(16)
Cd(11)-O(4)	2.638(10)	B(11)-O(30)#10	1.386(16)
Cd(12)-O(13)	2.196(11)	B(11)-O(13)	1.397(17)
Cd(12)-O(1)	2.242(9)	B(12)-O(21)	1.320(18)
Cd(12)-O(13)#2	2.268(11)	B(12)-O(29)#1	1.408(16)
Cd(12)-O(3)#1	2.291(9)	B(12)-O(26)#12	1.437(17)

O(23)#8-B(1)-O(7)	122.1(12)	O(27)#13-B(7)-O(24)#10	124.1(12)
O(23)#8-B(1)-O(29)	118.0(12)	O(27)#13-B(7)-O(18)	125.3(12)
O(7)-B(1)-O(29)	119.9(12)	O(24)#10-B(7)-O(18)	110.7(11)
O(11)#4-B(2)-O(6)	124.9(12)	O(15)#3-B(8)-O(1)	125.4(13)
O(11)#4-B(2)-O(24)	113.2(11)	O(15)#3-B(8)-O(17)	114.5(12)
O(6)-B(2)-O(24)	121.7(11)	O(1)-B(8)-O(17)	120.1(12)
O(12)-B(3)-O(8)	123.1(12)	O(9)-B(9)-O(25)	123.1(12)
O(12)-B(3)-O(28)	121.8(12)	O(9)-B(9)-O(26)	115.7(11)
O(8)-B(3)-O(28)	115.0(11)	O(25)-B(9)-O(26)	121.2(11)
O(3)-B(4)-O(20)#13	127.0(13)	O(19)-B(10)-O(4)	120.3(12)
O(3)-B(4)-O(18)	115.0(12)	O(19)-B(10)-O(2)	121.1(11)
O(20)#13-B(4)-O(18)	117.8(12)	O(4)-B(10)-O(2)	118.5(11)
O(5)-B(5)-O(17)	124.0(12)	O(16)-B(11)-O(30)#10	121.3(12)
O(5)-B(5)-O(28)	123.6(12)	O(16)-B(11)-O(13)	121.9(12)
O(17)-B(5)-O(28)	112.4(11)	O(30)#10-B(11)-O(13)	116.8(11)
O(22)-B(6)-O(10)	118.0(12)	O(21)-B(12)-O(29)#1	125.1(12)
O(22)-B(6)-O(14)#1	118.9(12)	O(21)-B(12)-O(26)#12	123.8(12)
O(10)-B(6)-O(14)#1	123.1(12)	O(29)#1-B(12)-O(26)#12	109.8(11)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1 #2 x,y,z+1 #3-x+1/2,-y,z+1/2

#4 -x+1/4,y+1/4,z-3/4 #5 -x,-y,z

#6 -x,-y,z-1 #7 x-1/4,-y+1/4,z+3/4

#8 -x+1/4,y-1/4,z+3/4 #9 -x+1/2,-y,z-1/2

#10 x+1/4,-y+1/4,z+1/4 #11 x+1/4,-y+1/4,z-3/4

#12 x-1/4,-y+1/4,z-1/4 #13 x+1/4,-y+1/4,z+9/4

Table S3. Calculation of local dipole moments for $Na_2Cd_7B_8O_{20}$, $Cd_2B_2O_5$ and $Cd_4BiO(BO_3)_3$.

Compounds	Species		Dipole moment			
			x(a)	y(b)	z(c)	debye
$Na_2Cd_7B_8O_{20}$	BO_3	$B(10)O_3$	0.26	-0.04	0.68	0.73
		$B(6)O_3$	0.18	-0.44	0.48	0.68
		$B(11)O_3$	0.91	-0.23	-0.16	0.95
	B_3O_7	$B(9)O_3$	0.04	-1.10	0.19	1.11
		$B(12)O_3$	-2.26	-2.65	1.46	3.78
		$B(1)O_3$	-0.64	0.07	-0.19	0.67
		B_3O_7	-2.86	-3.68	1.46	4.88
		$B(3)O_3$	0.30	-1.25	-0.11	1.29
		$B(5)O_3$	-0.87	-1.59	-0.22	1.82
		$B(8)O_3$	-1.37	-0.28	-0.94	1.68
		B_3O_7	-1.93	-3.12	-1.27	3.88
		$B(4)O_3$	0.97	-1.06	-1.82	2.32
		$B(7)O_3$	-0.88	-2.04	0.11	2.22
		$B(2)O_3$	-1.12	-0.73	1.16	1.77
		B_3O_7	-1.02	-3.83	-0.54	4.00
	NaO_4	$Na(5)O_4$	0	0	8.57	8.57
	NaO_6	$Na(6)O_6$	0.17	6.26	2.28	6.66
	Na/CdO_6	$Na(2)/Cd(3)O_6$	2.28	-2.37	-1.28	3.52
		$Na(3)/Cd(3)O_6$	3.58	5.23	1.38	6.48
	Na/CdO_5	$Na(1)/Cd(1)O_5$	-1.39	6.46	2.17	6.95
		$Na(4)/Cd(4)O_5$	-1.95	2.77	0.46	3.42
	CdO_6	$Cd(5)O_6$	2.85	1.95	1.65	3.83

		$Cd(7)O_6$	-1.42	-3.26	-1.02	3.69
		$Cd(8)O_6$	-2.15	6.07	-0.90	6.50
		$Cd(9)O_6$	0.78	-1.36	-0.78	1.75
		$Cd(10)O_6$	-1.21	0.98	0.05	1.56
		$Cd(12)O_6$	0.08	0.17	0.18	0.26
	CdO_7	$Cd(6)O_7$	-1.41	4.85	-1.38	5.23
		$Cd(11)O_7$	0.57	-3.45	0.77	3.59
$Cd_2B_2O_5$	CdO_6	$Cd(1)O_6$	-4.74	-2.33	-0.14	4.69
		$Cd(2)O_6$	3.12	5.18	2.47	5.76
		$Cd(3)O_6$	-4.08	-4.54	-2.22	5.59
		$Cd(4)O_6$	4.59	1.72	0.11	4.45
$Cd_4BiO(BO_3)_3$	CdO_6	$Cd(1)O_6$	1.18	-1.67	-0.30	2.10
	CdO_7	$Cd(2)O_7$	-3.19	2.84	-1.95	4.45