Electronic Supplementary Information (ESI) for:

$ACdCO_3F$ (A = K and Rb): new noncentrosymmetric materials with remarkably strong second-harmonic generation (SHG) responses enhanced via π-interaction

Guohong Zou,[a] Gnu Nam,[b] Hyung Gu Kim,[a] Hongil Jo,[a] Tae-Soo You,[b,*] and Kang Min Ok[a,*]

[a]Department of Chemistry, Chung-Ang University, Seoul, 156-756, Republic of Korea
[b]Department of Chemistry, Chungbuk National University, Cheongju, Chungbuk, 361-763, Republic of Korea.

*Corresponding Author:
Professor Kang Min Ok
Fax: +82-2-825-4736; Tel: +82-2-820-5197; E-mail: kmok@cau.ac.kr

Table S1. Atomic coordinates and displacement parameters for $KCdCO_3F$.

atom	*x*	*y*	*z*	U_{iso}
Cd(1)	0	0	0.5	0.01706
K(1)	0.6667	0.3333	0	0.01433
C(1)	0.3333	0.6667	0.5	0.01974
F(1)	0	0	0	0.01574
O(1)	0.4743(3)	0.5257(3)	0.5	0.02088

Table S2. Atomic coordinates and displacement parameters for $RbCdCO_3F$.

atom	*x*	*y*	*z*	U_{iso}
Cd(1)	0	0	0.5	0.01104
K(1)	0.6667	0.3333	0	0.01372
C(1)	0.3333	0.6667	0.5	0.01115
F(1)	0	0	0.	0.02637
O(1)	0.4724(4)	0.5276(4)	0.5	0.02522

Table S3. Selected bond lengths (Å) and angles (deg) for $KCdCO_3F$.

Cd1—F1	2.2139(9)	K1—F1	2.9612(12)
Cd1—O1	2.5742(10)	K1—O1	2.7967(9)
C1—O1	1.2524(5)	Cd1—K1—O1	90.87(3)
Cd1—K1—F1	113.609(5)	F1—K1—F1	120
K1—F1—K1	120	O1—C1—O1	120.00(2)

Table S4. Selected bond lengths (Å) and angles (deg) for $RbCdCO_3F$.

Cd1—F1	2.2646(9)	Rb1—F1	3.0082(12)
Cd1—O1	2.6167(10)	Rb1—O1	2.8641(8)
C1—O1	1.2549(5)	Cd1—Rb1—O1	90.767(3)
Cd1—Rb1—F1	113.548(5)	F1—Rb1—F1	120
Rb1—F1—Rb1	120	O1—C1—O1	120.00(2)

Fig. S1. Powder X-ray diffraction patterns for the thermal decomposition products of $KCdCO_3F$ (red line) and $RbCdCO_3F$ (green line).

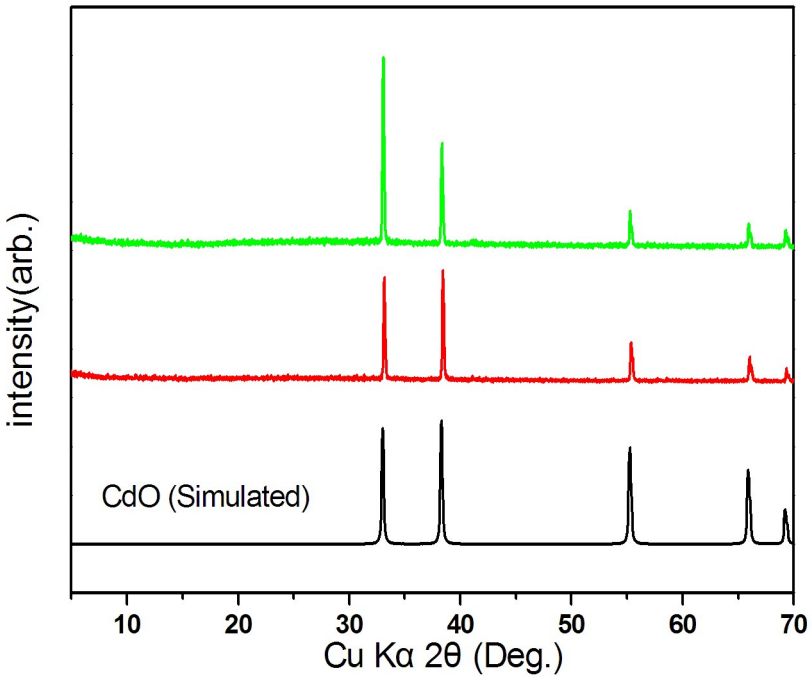

Fig. S2. IR spectra of $KCdCO_3F$ and $RbCdCO_3F$

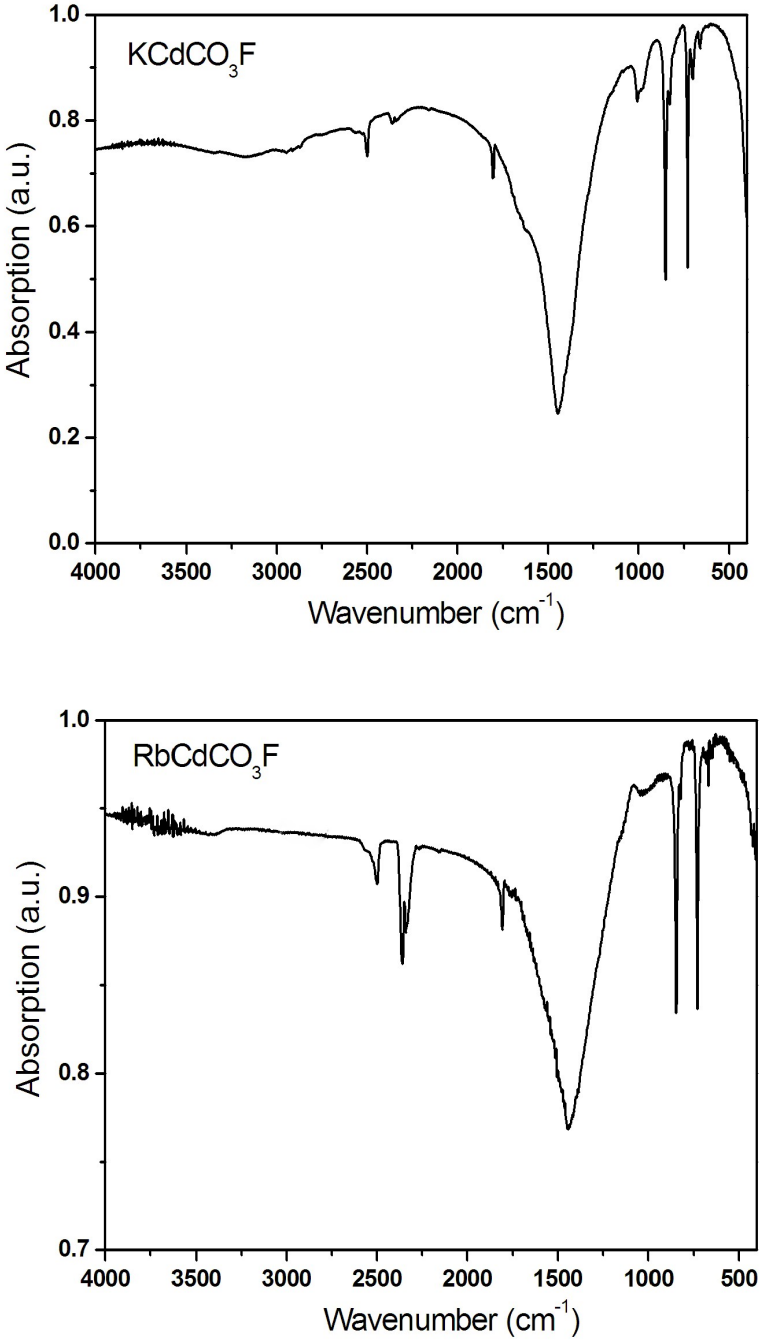

Fig. S3 Selected COHP curves of $KCdCO_3F$ representing (a) the C-O interaction in the $[CO_3]^{2-}$ unit, (b) the Cd-C and (c) the Cd-O interactions on the $[Cd(CO_3)]$ layer. E_F is indicated as the vertical dashed line and the energy reference (0 eV).