

## Supporting Information

### Synthesis, Crystal Structure and Optical Properties of a New Fluorocarbonate with Interesting Sandwich-like Structure

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#### Crystallographic information

The Crystallographic data for  $\text{Na}_3\text{Zn}_2(\text{CO}_3)_3\text{F}$  has been deposited with CCDC  
numbers of 1419125.

**Table S1.** Crystal data and structure refinement for  $\text{Na}_3\text{Zn}_2(\text{CO}_3)_3\text{F}$ 

$\text{Na}_3\text{Zn}_2(\text{CO}_3)_3\text{F}$	
Fw	398.74
$a(\text{\AA})$	14.6090(15)
$b(\text{\AA})$	8.5274(7)
$c(\text{\AA})$	20.1877(13)
$\beta$	102.426(7)
Space group	$C2/c$
$V(\text{\AA}^3)$	2456.0(4)
$Z$	12
$T(\text{K})$	103.5
$\lambda(\text{\AA})$	0.71073
$\rho_c(\text{g/cm}^3)$	3.236
$\mu(\text{cm}^{-1})$	6.081
$R(F)^a$	0.0438(1982)
$R_w(F_o^2)^b$	0.1150(2421)

**Table S2.** Selected bond lengths (Å) for Na<sub>3</sub>Zn<sub>2</sub>(CO<sub>3</sub>)<sub>3</sub>F

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Zn1–O9	1.984(4)	Zn3–O10	2.092(3)	O7–C3	1.280(5)
Zn1–O4	2.015(3)	Na1–F1	2.397(2)	O9–C3	1.281(5)
Zn1–O1	2.016(3)	Na1–F2	2.398(3)	C4–O11	1.248(5)
Zn2–O6	2.028(3)	Na2–F2	2.357(3)	C4–O10	1.307(5)
Zn1–O15	2.114(6)	Na2–F2	2.357(3)	C4–O12	1.307(5)
Zn1–O14	2.125(6)	C1–O1	1.280(5)	C5–O14	1.236(6)
Zn2–O8	1.996(3)	C1–O2	1.282(5)	C5–O13	1.295(6)
Zn2–O3	2.019(3)	C1–O3	1.281(5)	C5–O15	1.342(6)
Zn2–O12	2.089(3)	C2–O5	1.276(5)	Zn1–F2	2.041(2)
Zn3–O7	1.992(3)	C2–O6	1.282(5)	Zn2–F2	2.045(2)
Zn3–O2	2.022(3)	C2–O4	1.293(5)	Zn3–F1	2.0440(11)
Zn3–O5	2.022(3)	C3–O8	1.286(5)		

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**Table S3.** Positional coordinates and equivalent isotropic displacement parameters for Na<sub>3</sub>Zn<sub>2</sub>(CO<sub>3</sub>)<sub>3</sub>F.

Atom	Wyck.	Site	S.O.F.	x/a	y/b	z/c	U <sub>eq</sub> [Å <sup>2</sup> ]
Zn1	8f	1	1	0.19292(4)	0.27228(7)	0.34666(2)	0.00792(19)
Zn2	8f	1	1	0.13619(3)	0.27578(6)	0.14991(2)	0.00641(18)
Zn3	8f	1	1	0.02503(3)	-0.23285(6)	0.34978(2)	0.00618(18)
Na1	8f	1	1	0.14639(12)	-0.0414(2)	0.24981(8)	0.0107(4)
Na2	4e	2	1	0	0.4090(3)	1/4	0.0103(5)
Na3	8f	1	1	0.23474(11)	-0.0571(2)	0.43302(8)	0.0096(4)
Na4	8f	1	1	0.05478(13)	0.4409(2)	0.44546(10)	0.0191(5)
Na5	8f	1	1	0.38170(12)	0.4047(2)	0.42984(9)	0.0117(4)
F1	4e	2	1	0	-0.1682(4)	1/4	0.0111(8)
F2	8f	1	1	0.12599(17)	0.2377(3)	0.24805(11)	0.0102(6)
C1	8f	1	1	0.0338(3)	0.1027(5)	0.3640(2)	0.0074(9)
C2	8f	1	1	0.3529(3)	0.1019(5)	0.3261(2)	0.0067(9)
C3	8f	1	1	0.3062(3)	0.1066(5)	0.1533(2)	0.0091(10)
C4	8f	1	1	0.0887(3)	0.7585(5)	0.49889(19)	0.0096(11)
C5	4d	-1	1	1/4	1/4	1/2	0.0114(15)
O1	8f	1	1	0.1195(2)	0.0800(3)	0.36144(14)	0.0089(6)
O2	8f	1	1	-0.02241(19)	-0.0139(3)	0.36109(14)	0.0075(6)
O3	8f	1	1	0.0038(2)	0.2423(4)	0.36927(16)	0.0123(7)
O4	8f	1	1	0.3210(2)	0.2432(3)	0.32628(16)	0.0106(7)
O5	8f	1	1	0.4392(2)	0.0803(4)	0.32556(15)	0.0091(6)
O6	8f	1	1	0.29826(19)	-0.0155(3)	0.32687(14)	0.0070(6)
O7	8f	1	1	0.3381(2)	0.2437(4)	0.14555(16)	0.0098(7)
O8	8f	1	1	0.21966(19)	0.0886(4)	0.15592(14)	0.0065(6)
O9	8f	1	1	0.3603(2)	-0.0130(4)	0.1576(2)	0.0251(9)
O10	8f	1	1	0.0209(2)	0.7103(4)	0.44987(14)	0.0112(7)
O11	8f	1	1	0.1258(2)	0.8903(4)	0.49899(14)	0.0136(7)

O12	8f	1	1	0.1143(2)	0.6575(4)	0.54814(14)	0.0111(7)
O13	8f	1	0.5	0.1813(4)	0.3367(7)	0.5097(3)	0.0096(13)
O14	8f	1	0.5	0.2746(4)	0.2314(7)	0.4457(3)	0.0078(13)
O15	8f	1	0.5	0.2847(4)	0.1522(7)	0.5514(3)	0.0125(14)

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