

Electronic Supplementary Information (ESI) for:

Synthesis and Characterization of CsSrCO₃F – A Beryllium-Free New Deep-Ultraviolet Nonlinear Optical Material

Qingfei Li,^{a,b} Guohong Zou,^{*b} Chensheng Lin^c and Ning Ye^{*c}

^aInstitute of Atomic and Molecular Physics, Sichuan University, Chengdu, 610065, P. R. China.

^bInstitute of Chemical Materials and Advanced Materials Research Center, Key Laboratory of Science and Technology on High Energy Laser, China Academy of Engineering Physics, Mianyang, 621900, P. R. China.

^cFujian Institute of Research on the Structure of Matter, Key Laboratory of Optoelectronic Materials Chemistry and Physics, Chinese Academy of Sciences, Fuzhou, 350002, P. R. China.

CONTENTS

Table S1. Atomic coordinates and displacement parameters for CsSrCO₃F.

Table S2. Selected bond lengths (Å) and angles (deg) for CsSrCO₃F.

Figure S1. Powder X-ray diffraction patterns for CsSrCO₃F (black line) and the thermal decomposition products of CsSrCO₃F (red line).

Figure S2. IR spectrum of CsSrCO₃F.

Figure S3. Calculated band structure of CsSrCO₃F.

Table S1. Atomic coordinates and equivalent isotropic displacement parameters for CsSrCO₃F.

atom	x	y	z	U _{eq} (Å ²)	BVS
Sr1	0	0.6143(2)	1.0000	0.008(1)	2.349
Cs1	0.2798(1)	1.0000	0.5000	0.012(1)	0.991
F1	0	0.6172(5)	1.5000	0.017(1)	0.996
O(1)	0	0.8619(7)	1.0000	0.016(1)	2.031
O(2)	-0.3118(6)	0.4816(5)	1.0000	0.014(1)	2.190
C(1)	-0.3333	0.3333	1.0000	0.009(2)	3.952
C(2)	0	1.0000	1.0000	0.012(3)	3.674

Table S2. Selected bond lengths (Å) and angles (deg) for CsSrCO₃F.

Sr1—F1	2.375(9)	Cs1—F1	3.270(2)
Sr1—O1	2.393(1)	Cs1—O1	3.335(4)
Sr1—O2	2.529(2)	Cs1—O2	3.238(3)
C2—O1	1.3153(5)	C1—O2	1.289(1)
Cs1—F1—Cs1	134.263(2)	F1—Cs1—F1	148.525(4)
O2—C1—O2	120.00(4)	O1—C2—O1	120.00(2)

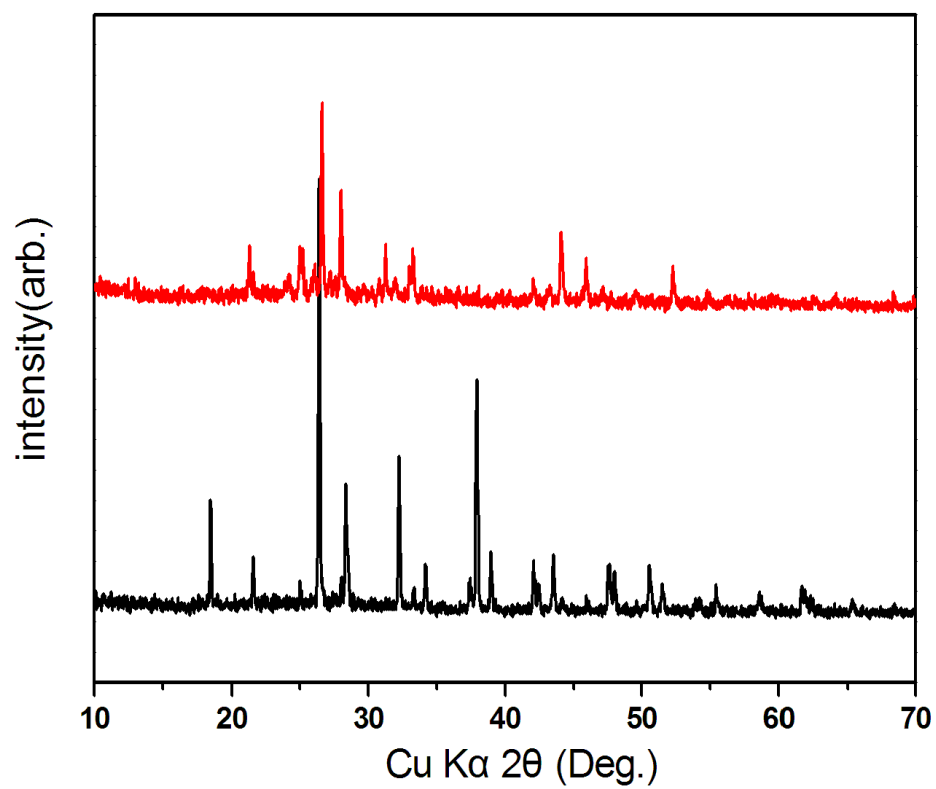


Figure S1. Powder X-ray diffraction patterns for CsSrCO₃F (black line) and the thermal decomposition products of CsSrCO₃F (red line).

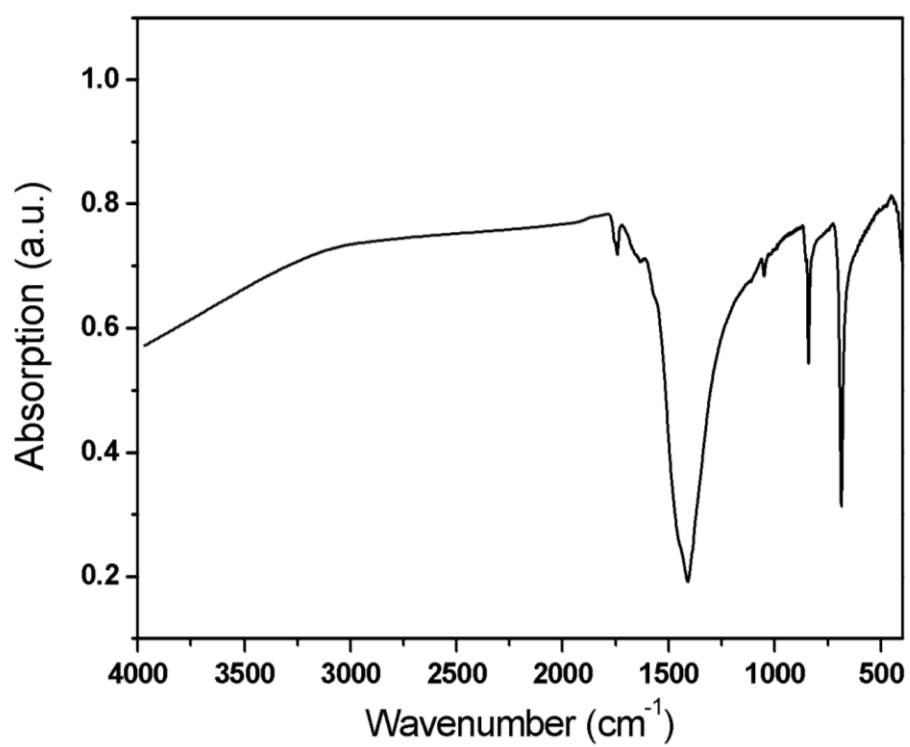


Figure S2. IR spectrum of CsSrCO₃F.

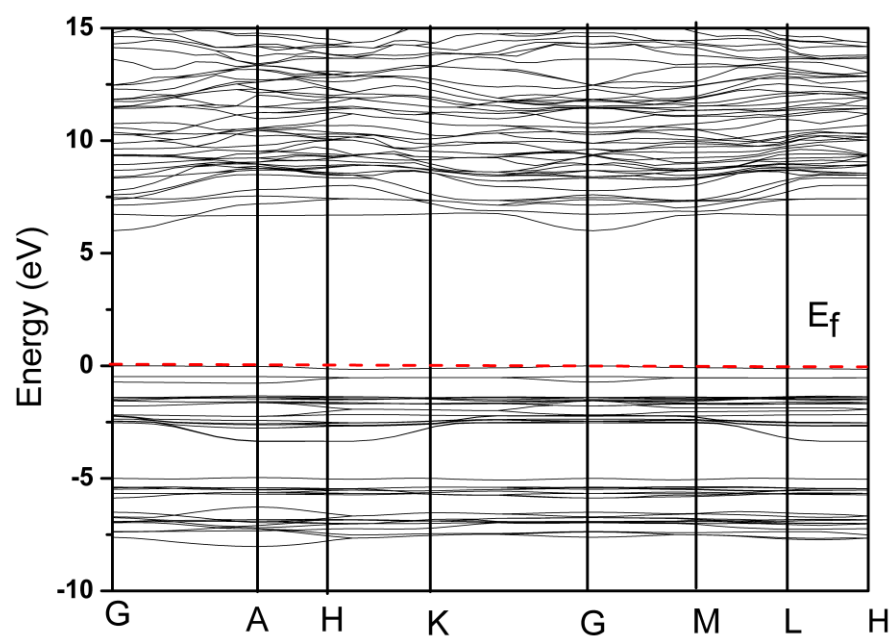


Figure S3. Calculated band structure of CsSrCO₃F (the Fermi level is set at 0 eV).