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Supporting information for article:

Synthesis, structure and NLO properties of a new isostructural β -d-fructopyranose alkaline halide MOFs: a theoretical and experimental study

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Supporting information

Table S1 Hydrogen bond distances for compounds **CaFRUCl**, **CaFRUBr**, **SrFRUCl** and **SrFRUBr**.
X=Cl, Br.

D-H...A (Å) D...A (Å) D-H...A (°)	CaFRUCl	CaFRUBr	SrFRUCl	SrFRUBr
H1WB...X ⁱ	2.14	2.40	2.27	2.42
O1W...X ⁱ	3.0967(3)	3.241(3)	3.114(3)	3.251(4)
O1W-H1WB...X ⁱ	175	179	174	163
H2...X	2.30	2.45	2.26	2.46
O2...X	3.1336(3)	3.293(4)	3.120(3)	3.277(5)
O2-H2...X	171	173	154	163
H1WA...O5 ⁱⁱ	1.97	2.03	2.00	2.09
O1W...O5 ⁱⁱ	2.8628(2)	2.880(6)	2.836(5)	2.828(7)
O1W- H1WA...O5 ⁱⁱ	160	178	167	156
H2W...X	2.14	2.38	2.24	2.35
O2W...X	3.0650(3)	3.193(3)	3.052(3)	3.203(3)
O2W-H2W...X	168	163	154	180
H3...O4 ⁱⁱⁱ	1.97	2.00	2.06	2.01
O3...O4 ⁱⁱⁱ	2.7667(2)	2.780(5)	2.756(5)	2.777(7)
O3-H3...O4 ⁱⁱⁱ	161	152	131	152
H4...X ^{iv}	2.27	2.41	2.70	2.83
O4...X ^{iv}	3.0774(3)	3.225(3)	3.101(3)	3.243(4)
O4-H4...X ⁱⁱⁱ	175	170	112	113
H5...O2W ^v	1.88	1.88	2.29	1.88
O5...O2W ^v	2.6934(2)	2.695(4)	2.714(5)	2.692(5)
O5-H5...O2W ^v	169	172	111	171
H6...X	2.70	2.89	2.59	2.76
O6...X	3.4686(3)	3.673(4)	3.392(4)	3.551(5)
O6-H6...X	162	161	158	162
H6...O1	2.29	2.26	2.30	2.27
O6...O	2.6942(2)	2.691(5)	2.690(4)	2.697(6)
O6-H6...O1	112	113	108	113
H6B...O4 ^{vi}	2.48	2.48	2.57	2.59
C6...O4 ^{vi}	3.3344(3)	3.314(6)	3.428(7)	3.448(8)
C6-H6B...O4 ^{vi}	148	145	147	147

Symmetry operations: i) $x, -1+y, z$; ii) $-0.5+x, -0.5+y, 0.5+z$; iii) $0.5-x, -0.5+y, 0.5-z$; iv) $-x, y, -z$; v) $0.5+x, 0.5+y, 0.5+z$; vi) $0.5-x, 0.5+y, 0.5-z$

Figure S1 Powder patterns of **CaFRUCI**, collected before (black) and after (blue) irradiation for SHG measurements. Powder patterns calculated from the X-ray determined structures were reported in red.

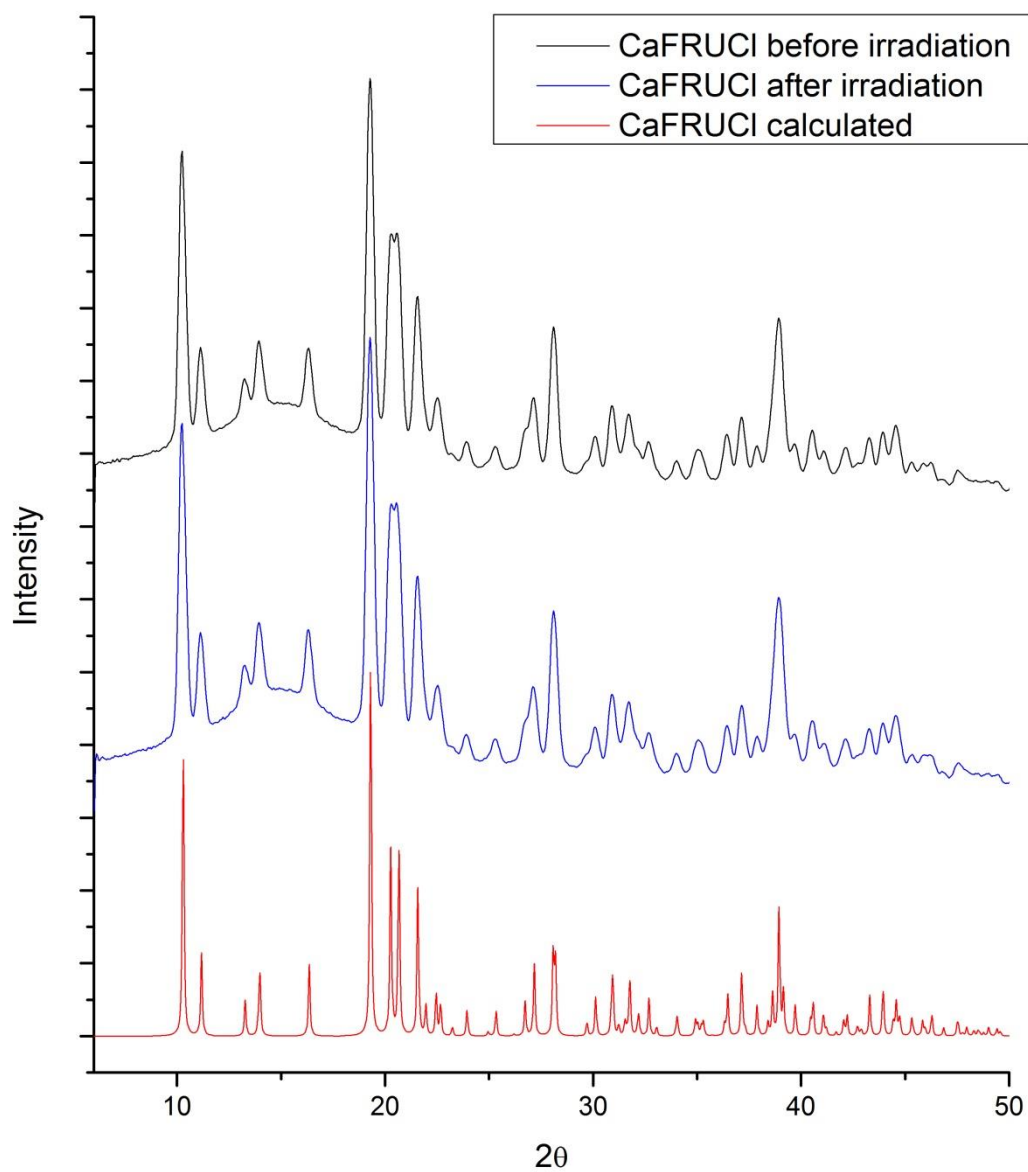


Figure S2 Powder patterns of **CaFRUBr** collected before (black) and after (blue) irradiation for SHG measurements. Powder patterns calculated from the X-ray determined structures were reported in red.

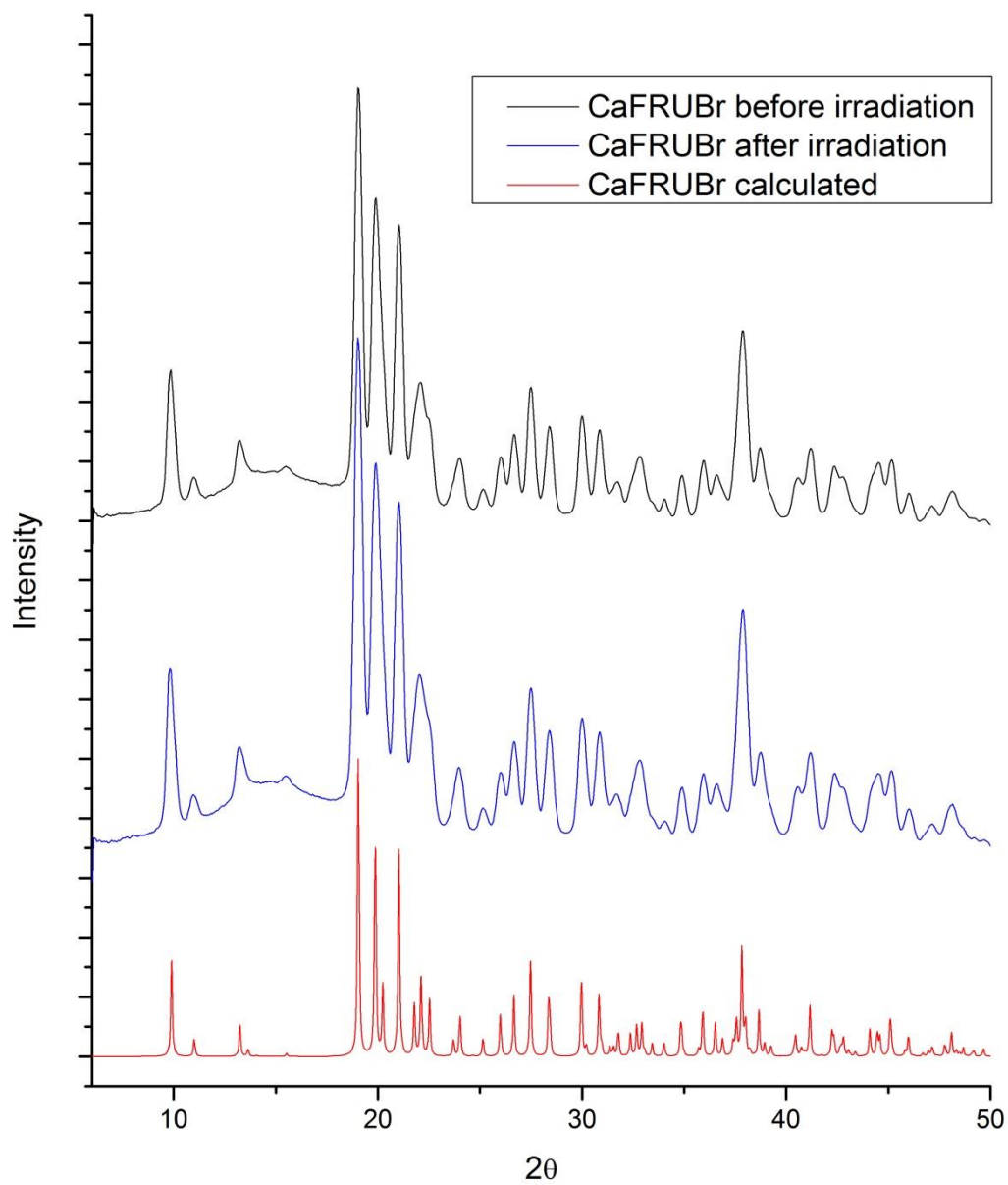


Figure S3 Powder patterns of **SrFRUCI**, collected before (black) and after (blue) irradiation for SHG measurements. Powder patterns calculated from the X-ray determined structures were reported in red.

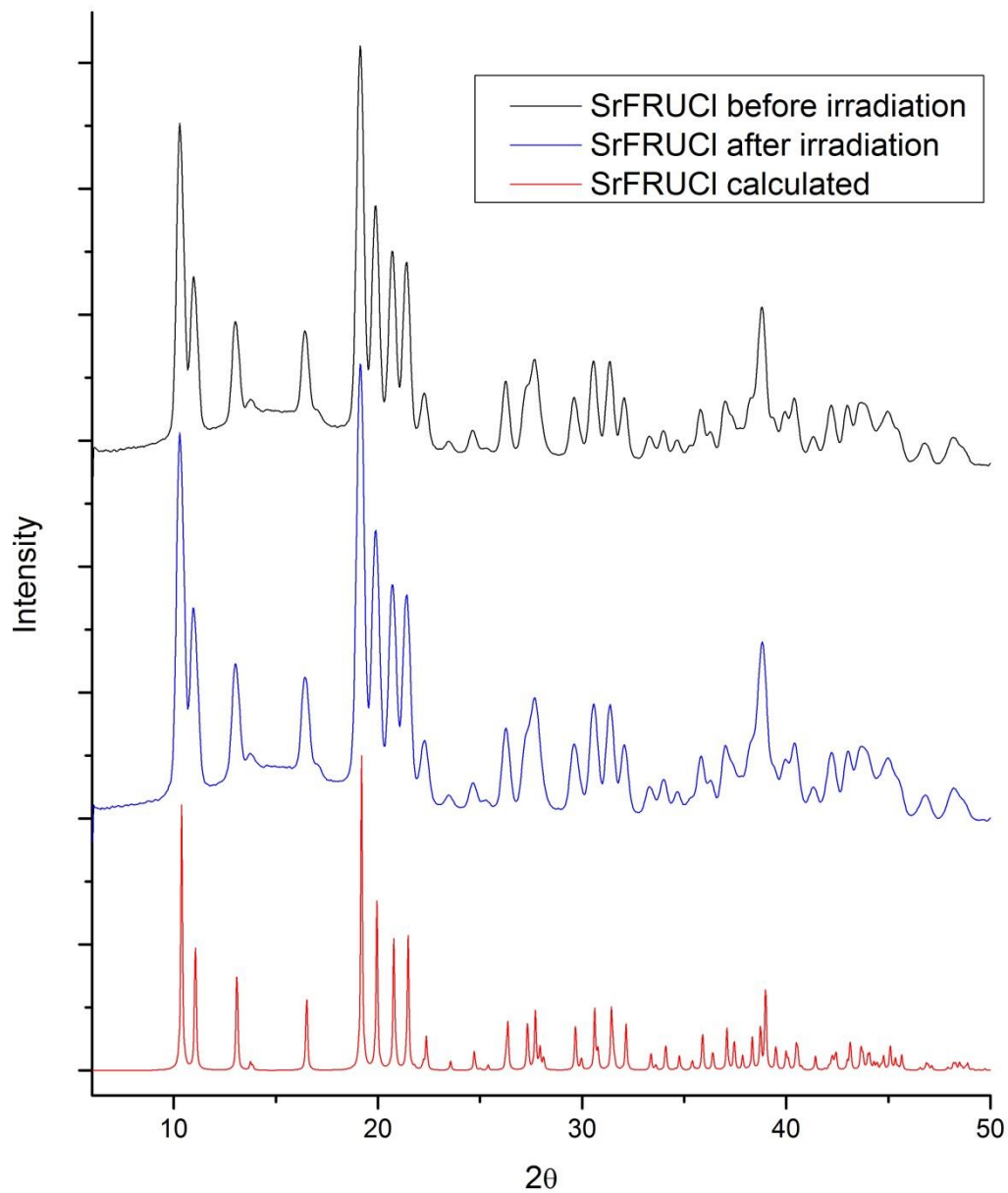


Figure S4 Powder patterns of **SrFRUBr** collected before (black) and after (blue) irradiation for SHG measurements. Powder patterns calculated from the X-ray determined structures were reported in red.

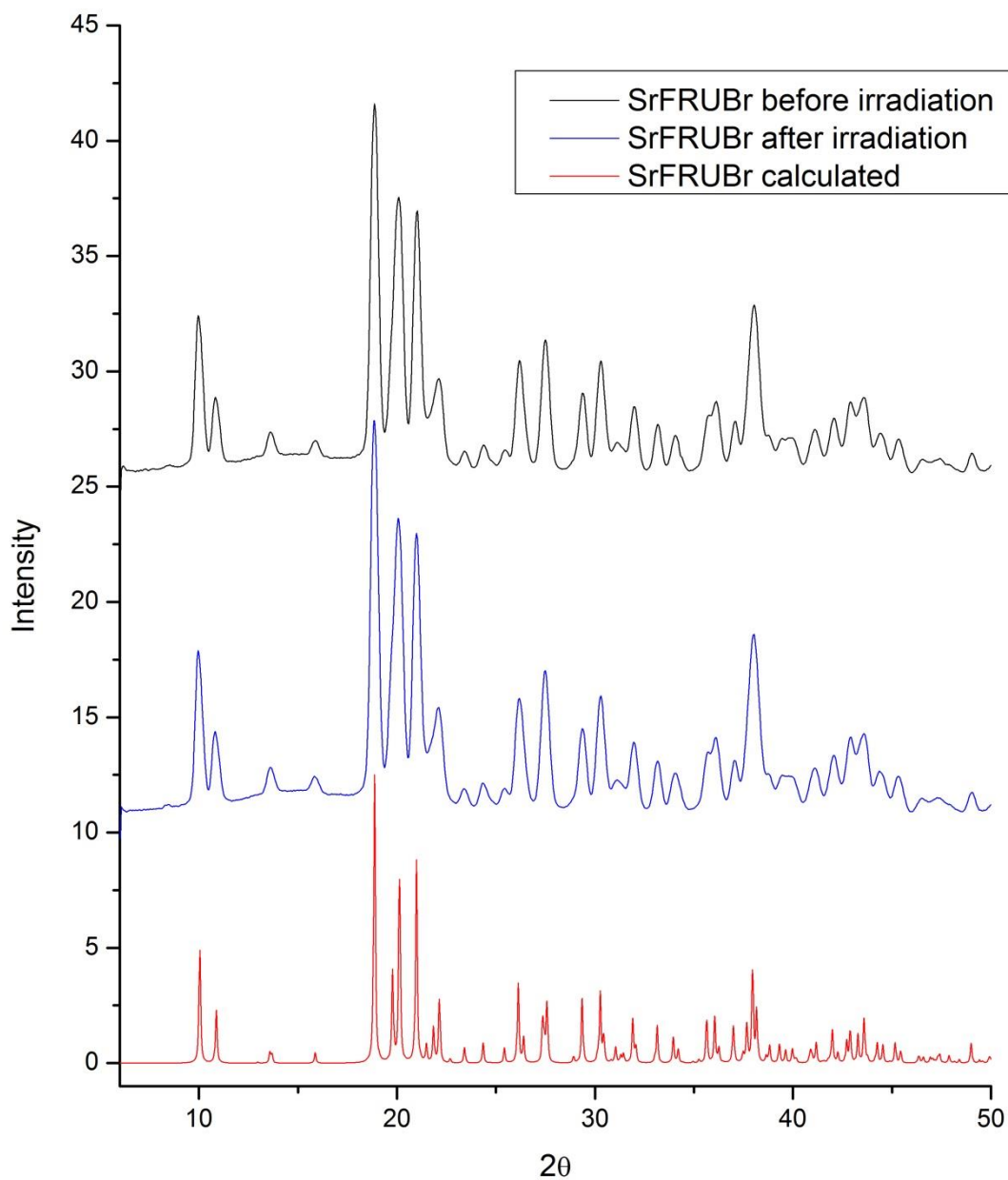


Figure S5 FT-infrared spectra of **CaFruCl** sample before and after irradiation in the SHG measurements. Signal intensity (*I*) is in arbitrary units (a.u.).

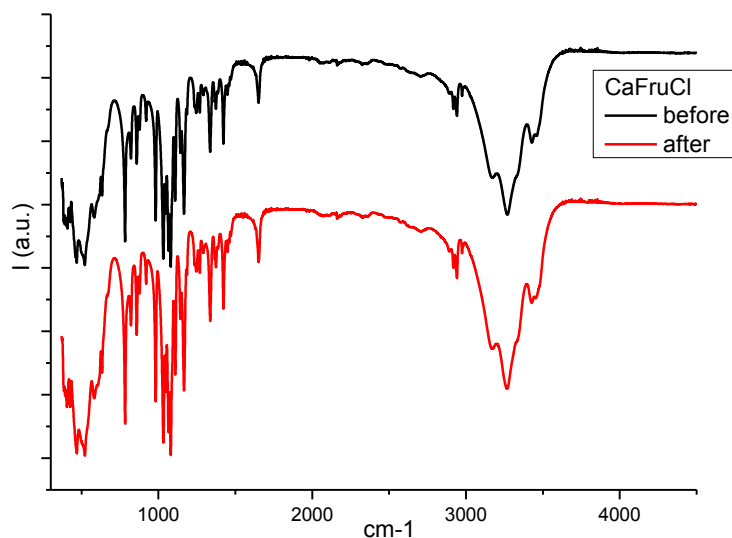


Figure S6 FT-infrared spectra of **CaFruBr** sample before and after irradiation in the SHG measurements. Signal intensity (*I*) is in arbitrary units (a.u.).

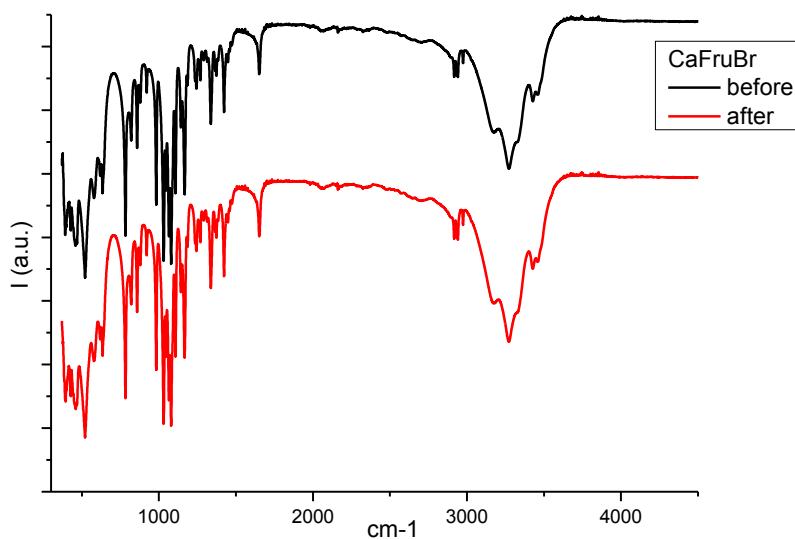


Figure S7 FT-infrared spectra of **SrFruCl** sample before and after irradiation in the SHG measurements. Signal intensity (*I*) is in arbitrary units (a.u.).

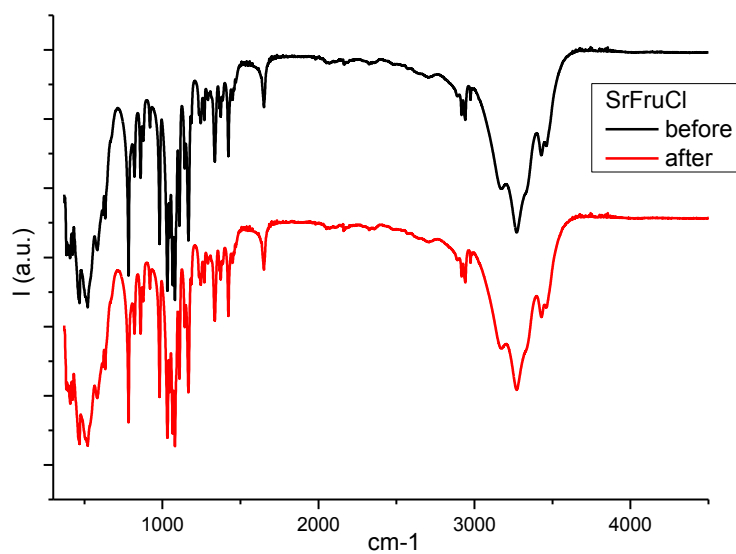


Figure S8 FT-infrared spectra of **SrFruBr** sample before and after irradiation in the SHG measurements. Signal intensity (*I*) is in arbitrary units (a.u.).

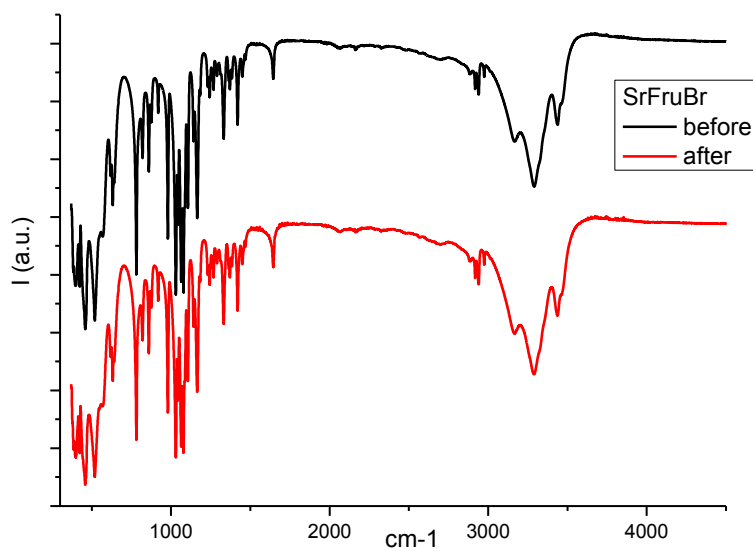


Figure S9 FT-Raman spectra of **CaFruCl** sample before and after irradiation in the SHG measurements. Signal intensity (I) is in arbitrary units (a.u.).

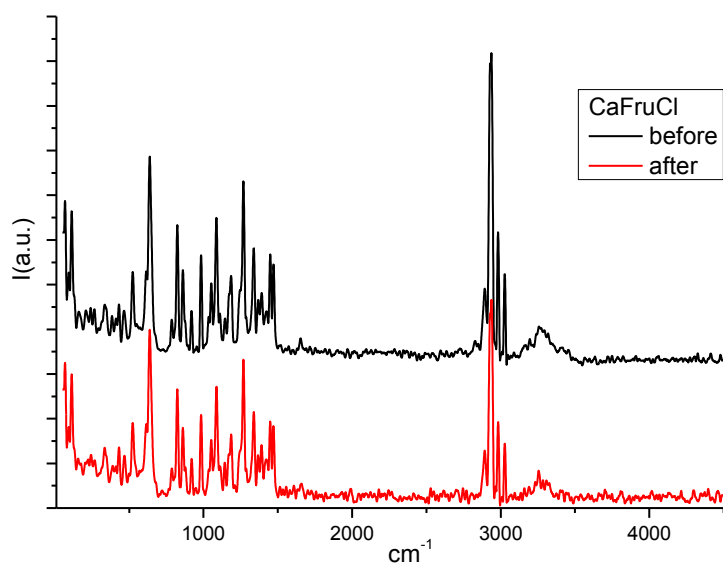


Figure S10 FT-Raman spectra of **CaFruBr** sample before and after irradiation in the SHG measurements. Signal intensity (I) is in arbitrary units (a.u.).

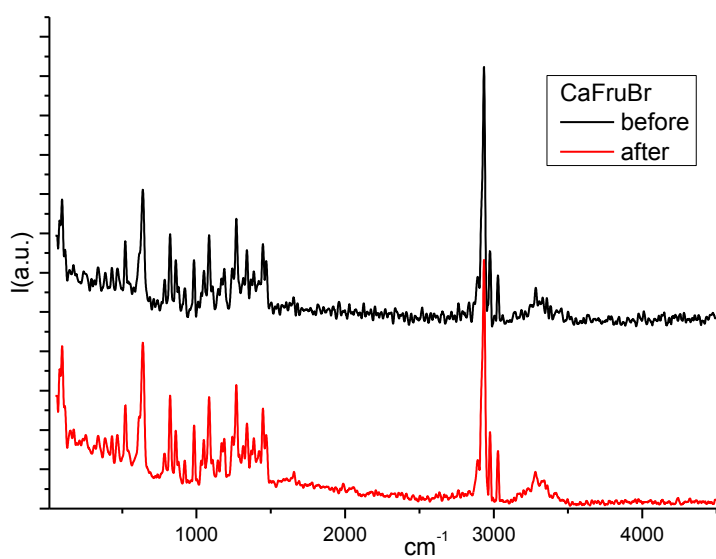


Figure S11 FT-Raman spectra of **SrFruCl** sample before and after irradiation in the SHG measurements. Signal intensity (*I*) is in arbitrary units (a.u.).

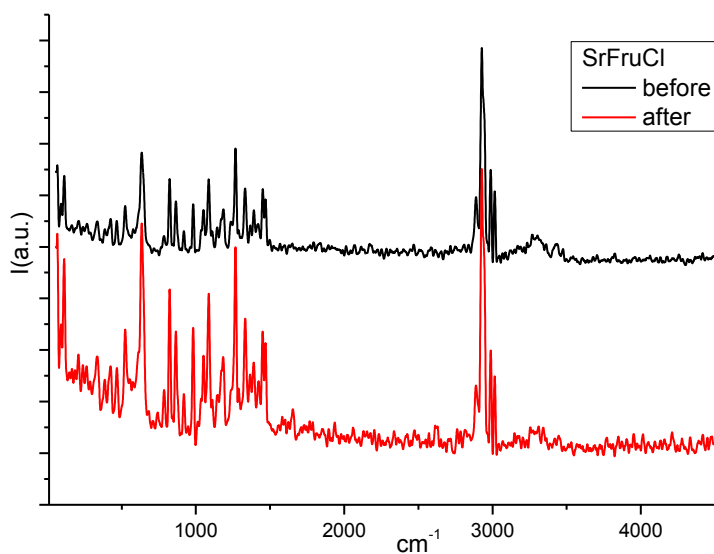


Figure S12 FT-Raman spectra of **SrFruBr** sample before and after irradiation in the SHG measurements. Signal intensity (*I*) is in arbitrary units (a.u.).

