Title:	A series of s-block (Ca, Sr and Ba) metal–organic frameworks: synthesis and structure–property correlation
Authors:	Sirohi, Anshu (/jspui/browse?type=author&value=Sirohi%2C+Anshu) Yadav, Lalit (/jspui/browse?type=author&value=Yadav%2C+Lalit) Sheet, G. (/jspui/browse?type=author&value=Sheet%2C+G.)
Keywords:	Metal–organic framework Ca, Sr and Ba Pentameric clusters Space group
Issue Date:	2016
Publisher:	Royal Society of Chemistry
Citation:	CrystEngComm, 18(6), pp. 1046-1053
Abstract:	A series of metal–organic frameworks based on alkaline earth metal ions (Ca, Sr and Ba) and 1,3,5-benzenetribenzoic acid (BTB) have been synthesized and characterized. These are [H2N(CH3)2][Ca7(BTB)5(H2O)8(DMF)4]·4H2O (1), [H2N(CH3)2]2[Sr5(H2O)6(BTB)4] (2) and [H2N(CH3)2][Ba(H2O)(BTB)] (3). All the structures are three-dimensional in nature with different secondary building units. Compound 1 contains one-dimensional Ca–O–Ca zigzag chains while compound 2 contains Sr5O28 pentameric clusters and compound 3 contains one-dimensional Ba–O–Ba chains. Both compounds 1 and 3 form (3,6)-net connectivity while compound 2 forms (3,12)-net connectivity. Optical band gap energy measurements show that compound 1 (2.65 eV) has low band gap energy compared to 2 (3.22 eV) and 3 (3.32 eV). This variation in band gap energy may be due to the difference in structural arrangement. Compound 3 crystallizes in a non-centrosymmetric space group (Pna21), which belongs to the polar point group C2v. This compound displays a strong SHG response and good ferroelectric and piezoelectric properties.
Description:	Only IISERM authors are available in the record.
URI:	https://pubs.rsc.org/en/Content/ArticleLanding/CE/2016/C5CE01995H#!divAbstract (https://pubs.rsc.org/en/Content/ArticleLanding/CE/2016/C5CE01995H#!divAbstract) http://hdl.handle.net/123456789/2543 (http://hdl.handle.net/123456789/2543)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/2543/1/Need%20to%20add%20pdf.odt)		7.9 kB	OpenDocument Text	View/Open (/jspui/bitstream/12345

Show full item record (/jspui/handle/123456789/2543?mode=full)
(/jspui/handle/123456789/2543/statistics)