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Title:	Unusual crystallographic existence of a hydrated zinc(ii) bisulphate complex: Experimental and theoretical observations
Authors:	Yadav, H.R. (/jspui/browse?type=author&value=Yadav%2C+H.R.) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	hydrated zinc(ii) bisulphate complex [Zn(H <sub>2</sub> O) <sub>6</sub> ](HSO <sub>4</sub> ·H <sub>2</sub> O) <sub>2</sub> (1)
Issue Date:	2015
Publisher:	Royal Society of Chemistry
Citation:	RSC Advances, 5(53) pp. 42681-42688
Abstract:	A unprecedented hydrated zinc(ii) bisulphate complex, [Zn(H <sub>2</sub> O) <sub>6</sub> ](HSO <sub>4</sub> ·H <sub>2</sub> O) <sub>2</sub> (1) has been synthesized along with a molecular ion salt, [4,4'-bipy-H <sup>+</sup> ][NCS <sup>-</sup> ] (2) (4,4'-bipy = 4,4'-bipyridine) and characterized by different spectroscopic tools including a single crystal X-ray diffraction study. From the X-ray crystal structure of 1, it is revealed that the Zn(ii) ion is in a perfect octahedral geometry with a ZnO <sub>6</sub> core and the molecule crystallizes in the P21/c space group. Self-assembly of the bisulphate anions with lattice water molecules pack to form a 12-membered cyclic cluster through strong intermolecular H-bonding (O-H...O-S). Again four cyclic tetramers interact with one another via H...O bonding to form a 20-membered macrocyclic bisulphate-water cluster and extends as a 2D network along the a axis. It presents a new mode of association of water molecules with bisulphate molecules. Density Function Theory (DFT) studies agree well with the experimental findings
Description:	Only IISERM authors are available in the record.
URI:	<a href="https://pubs.rsc.org/en/content/articlelanding/2015/ra/c5ra02640g#!divAbstract">https://pubs.rsc.org/en/content/articlelanding/2015/ra/c5ra02640g#!divAbstract</a> ( <a href="https://pubs.rsc.org/en/content/articlelanding/2015/ra/c5ra02640g#!divAbstract">https://pubs.rsc.org/en/content/articlelanding/2015/ra/c5ra02640g#!divAbstract</a> ) <a href="http://hdl.handle.net/123456789/3089">http://hdl.handle.net/123456789/3089</a> ( <a href="http://hdl.handle.net/123456789/3089">http://hdl.handle.net/123456789/3089</a> )
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