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Title:	Structure and stability of water chains (H ₂ O) _n , n = 5-20
Authors:	Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	Atoms-in-molecules Bond critical points Helical chains Equations of state Hydrogen Hydrogen bonds, Water analysis
Issue Date:	2009
Publisher:	American Chemical Society
Citation:	Journal of Physical Chemistry A, 113 (16), pp. 3744-3749.
Abstract:	The structure and stability of linear (helical) water chains (H ₂ O) _n , n = 5-20 as obtained from ab initio/DFT calculations are reported along with an atoms-in-molecules (AIM) analysis of hydrogen bond critical points and their characteristics. The resulting helical chain arrangement is one of the predominant motifs in different host environments; although they may not be the most stable, it is shown that these linear water chain clusters could exist in their own right.
Description:	Only IISERM authors are available in the record.
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