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Title:	Disruptive influence of the host cage C60 on the guest He-H+ bond and bonding in H3+
Authors:	Sathyamurthy, Narayanasami (/jspui/browse?type=author&value=Sathyamurthy%2C+Narayanasami)
Keywords:	He-H+ host cage C60
Issue Date:	2021
Publisher:	Elsevier
Citation:	Journal of the Indian Chemical Society, 98(8), 100101.
Abstract:	Although a helium atom prefers to stay at the centre of a fullerene (C60) cage and a proton binds with one of the carbon atoms from inside, DFT(MN15)/cc-pVTZ and DLPNO-MP2/def2-TZVP calculations show that the helium atom and the proton in HeH+ prefer to stay away from the centre of the cage, weakening the He-H+ covalent bond considerably. Both the helium atom and the proton exhibit noncovalent interactions with the carbon atoms of two pentagons at the opposite ends of the fullerene cage. Our calculations also show that a linear arrangement of H3+ (inside C60), pointing towards the centres of two pentagons opposite to each other, with the proton breaking away from H2, is energetically more favored over the equilateral triangle geometry of free H3+.
Description:	Only IISERM authors are available in the record.
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