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Title:	Stabilization of the C <sub>20</sub> cage by encapsulation of H <sup>+</sup> and He <sup>2+</sup> ions
Authors:	Abhijith Kumar, R.P.S. (/jspui/browse?type=author&value=Abhijith+Kumar%2C+R.P.S.) Dev, Sagarika (/jspui/browse?type=author&value=Dev%2C+Sagarika) Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	Atoms-in-molecules Encapsulation of protons Fullerene Natural bond orbital Perturbation theory
Issue Date:	2014
Publisher:	Indian Academy of Sciences
Citation:	Current Science, 106(9), pp.1255-1259.
Abstract:	It is shown by ab initio calculations using secondorder Møller-Plesset perturbation theory and 6-31g*, aug-cc-pVDZ and aug-cc-pVTZ basis sets and coupled cluster singles, doubles and perturbative triples method with the 6-31g* basis set, that it is possible to stabilize the cage structure of the smallest fullerene C <sub>20</sub> by encapsulating small cations like H <sup>+</sup> and He <sup>2+</sup> . While the latter stabilizes the cage structure by charge transfer, the former prefers to form a covalent linkage with the carbon atoms.
Description:	Only IISERM authors are available in the record.
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