Title:	Heat capacity of endohedral fullerenes Rg@C 60 (Rg = He, Ne, Ar and Kr)
Authors:	Koner, A. (/jspui/browse?type=author&value=Koner%2C+A.) Kumar, Chandan (/jspui/browse?type=author&value=Kumar%2C+Chandan) Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	Molar heat capacity endohedral fullerenes Hartree–Fock density functional theory harmonic oscillator three dimensional isotropic
Issue Date:	2018
Publisher:	Taylor and Francis Ltd.
Citation:	Molecular Physics, 116(19-20), pp. 2728-2735
Abstract:	The heat capacity of rare gas containing endohedral fullerenes has been computed by computing the vibrational frequencies of the molecules using the Hartree–Fock method and the density functional theoretic method with the wB97XD functional and the 6-31G* basis set. The consequences of the translational motion of the rare gas atom becoming vibrational motion inside the fullerene cavity are examined by comparing the computed vibrational frequencies for fullerene and the endohedral fullerenes. The increase in the heat capacity of the endohedral fullerenes due to encapsulation is interpreted in terms of the bound states of a three dimensional isotropic harmonic oscillator.
URI:	https://www.tandfonline.com/doi/full/10.1080/00268976.2018.1463468 (https://www.tandfonline.com/doi/full/10.1080/00268976.2018.1463468) http://hdl.handle.net/123456789/1757 (http://hdl.handle.net/123456789/1757)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/1757/1/Need%20to%20add%20pdf.odt)		8.04 kB	OpenDocument Text	View/Open (/jspui/bitstream/12345

Show full item record (/jspui/handle/123456789/1757?mode=full)
(/jspui/handle/123456789/1757/statistics)