

Density functional study of the Xe_2H_3^+ cation.

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A density functional theory investigation has been carried out to determine the equilibrium geometry, binding energy and vibrational properties of Xe_2H_3^+ . The molecule is a linear centrosymmetric species with a dissociation energy of $\sim 80 \text{ kJ mol}^{-1}$ corresponding to the dissociation limit of Xe_2H^+ and two hydrogen atoms. At the B3LYP/aug-cc-pVQZ level employing 18-VE effective core potential on xenon the terminal Xe–H bonds are predicted to be shorter ($1.7149 \text{ \AA}$) than the Xe–H bonds involving the center hydrogen ($2.1298 \text{ \AA}$). Computationally the most strongest vibrational band involves a Xe–H stretch of the center hydrogen inducing an extremely strong band at 1163 cm^{-1} . The bonding properties of Xe_2H_3^+ have been studied according to topological analysis of the electron localization function (ELF), which indicate that the terminal hydrogens are bound by covalent interactions. The center hydrogen is bound to the neighboring xenons mainly by electrostatic forces even though a non-negligible fraction of covalent nature is found.

Adres publiczny

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