Title:	Effect of confinement on ammonia inversion
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Abstract:	The effect of confinement on ammonia inversion inside C50 (D5h) and C60 (Ih) fullerenes has been investigated. Calculations at the DFT(M06-2X)/6-311G** level of theory suggest that NH3 is stable inside both C50 and C60 by −8.6 and −23.8 kcal mol−1, respectively. While the barrier for inversion of the free NH3 molecule is estimated to be 1896 cm−1, it increases to 1972 cm−1 and 2108 cm−1, respectively, inside C50 and C60. The results also reveal that the magnitude of splitting of the bound states below the barrier in the symmetric double-well potential decreases inside both the C50 and C60 cages.
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