

NMR Study of M@C₈₂ Anion

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Endohedral metallofullerenes (fullerenes with metal atoms encapsulated inside hollow carbon cages) have attracted special interest as new spherical molecules because they have unique properties that are not seen in empty fullerenes.¹ Among these, La@C₈₂ has been recognized as a prototype of endohedral metallofullerenes since its first extraction in 1991 by Smalley and co-workers.² We have verified that the carbon cages of the major (La@C₈₂-A) and minor (La@C₈₂-B) isomers of La@C₈₂ have C_{2v}³ and C_s⁴ symmetry, respectively, by analysis of the ¹³C NMR spectra of their anions. In this context, we applied this methodology for the structural determination of Pr@C₈₂⁵ and Ce@C₈₂,⁶ and also for the 2D NMR measurement.

References

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