

# Shielding cone behavior in the spherical aromatic He@C<sub>60</sub>: origin of the record for the most shielded encapsulated <sup>3</sup>He nucleus and comparison to He@C<sub>70</sub>

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The textbook concept of shielding cone is one of the characteristic properties for planar aromatic species, which explains the nuclear shielding of neighbor molecules located above and below the molecular plane. Here, we explore its resemblance in spherical aromatic fullerenes, where particularly for C<sub>60</sub>, it explains the record for the highest shielding observed via <sup>3</sup>He-NMR for the endohedral <sup>3</sup>He@C<sub>60</sub> species. Our results compare the behavior for He@C<sub>60</sub> and He@C<sub>60</sub> denoting relevant changes in their magnetic response behavior, where an induced shielding cone was observed for the latter with its long-range shielding character. In contrast to planar aromatics which give rise to a shielding cone property only for a perpendicularly oriented field, it was found that the shielding cone in spherical aromatic fullerenes occurs to any orientation. Thus, the orientation dependence behavior of the shielding cone is accounted, unraveling a characteristic shielding cone pattern in He@C<sub>60</sub> which further rationalizes its record on the most shielded He nucleus, upon rotation or tumbling from the aromatic ring about the applied field. For the C<sub>70</sub> case, the opposite situation has been characterized via <sup>3</sup>He-NMR experiments, which is explained in terms of the deshielding/shielding region inside the C<sub>70</sub> cage. [Figure not available: see fulltext.]. © 2019, Springer-Verlag GmbH Germany, part of Springer Nature.

<sup>3</sup>He-NMR

Shielding

Shielding cone

Spherical aromaticity

article

male

nuclear magnetic resonance

rotation