

***Interactive comment on* “EPR Study of NO radicals encased in modified open C60 Fullerenes” by Klaus-Peter Dinse et al.**

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We are grateful to the referee for the constructive and helpful comments on our manuscript. Below we respond point-by-point to the comments and include suggestions for corresponding revisions of the manuscript.

Referee 1 Malcom Levitt:

1) In the abstract, it is not very clear that the confining cage is not C60 but an open-cage variant (in fact two variants) of C60.

Response: The first sentence of the abstract will be rephrased: “... confined in two different modified open C60 derived cages are determined.” Further changes will be made in reply to Referee 2, 1).

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2) *In the introduction, references are given to some of the molecular endofullerenes produced by the Kyoto group and others, but some important systems of this kind are omitted, for example the water endofullerene (Murata and coworkers) and also the HF and CH₄ endofullerenes (Whitby and coworkers).*

Response: Three additional references will be included:

- a) K. Kurotobi and Y. Murata, *Science*, 2011, 333, 613–616 (H₂O@C₆₀)
- b) A. Krachmalnicoff et al., *Nature Chemistry*, 2016, 8(10) 953–957 (HF@C₆₀)
- c) S. Bloodworth et al., *Ang. Chem. Int. Ed.*, 2019, 58(15) 5038–5043 (CH₄O@C₆₀)

3) *The ball and stick graphics in Fig.1 do not depict the chemical structures of these compounds clearly enough. They should be supplemented by ChemDraw-style line structures showing clearly the chemical nature of the orifice and the appended groups.*

Response: Fig. 1 will be changed to display only NO@C₆₀-OH₁ with the left part as “side view” of the modified C₆₀ cage represented by true balls-and-sticks together with the caged NO represented by van-der-Waals spheres. The right part will show a “top view” onto the orifice with the orifice atoms represented by van-der-Waals spheres. The caged NO will again also be displayed as van-der-Waals spheres, but the modified C₆₀ cage represented only by sticks. NO@C₆₀-OH₃ will be shown as Fig. A1 in the appendix identical to the original Fig. 1b). We attach the new Fig. 1 Left (side view of NO@C₆₀-OH₁ as Fig. 1 to this comment.

4) *There are a few places where I felt that more references would be appropriate, especially for readers who are not highly conversant with EPR techniques. For example the PEANUT method is not referenced. No reference is given for the lambda value for NO (line after Eq.1). No explicit reference is given for the reported data on related systems (end of first paragraph on page 7).*

Response: References had been misplaced at several instances and will be given at the appropriate places, e.g. the PEANUT reference (Stoll et al., 1998) was misplaced

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at line 47 instead of line 45.

5) *It is not clear until quite late in the discussion that the hyperfine data refers to coupling to the ^{14}N nucleus.*

Response: This will be clarified by replacing the sentence starting at line 150 by:

“The frequency position at the low field side of the spectrum and the magnitude of the shift is inconsistent with proton hfi but is indicative for a dominant dipolar ^{14}N hfi, . . .”.

6) *A comparison with the observations reported on the similar O2 system (Futagoishi et al.) would have been interesting and enhance the manuscript.*

Response: This will be incorporated at line 99 after “. . . (200 K) is determined” by:

“The lifting of $^2\pi_x/{}^2\pi_y$ degeneracy is not unexpected considering the observation of a finite zero-field-splitting for ${}^3\text{O}_2$ in a cage with C_1 symmetry (Futagoishi et al., 2017). In this study the potential barrier for librational motions of ${}^3\text{O}_2$ was estimated as 398 cm^{-1} , by measuring the shift of its principal ZFS component with respect to the value of the free molecule. The size of this potential barrier is of the same order of magnitude as the one calculated for NO.”

Interactive comment on Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2020-11>, 2020.

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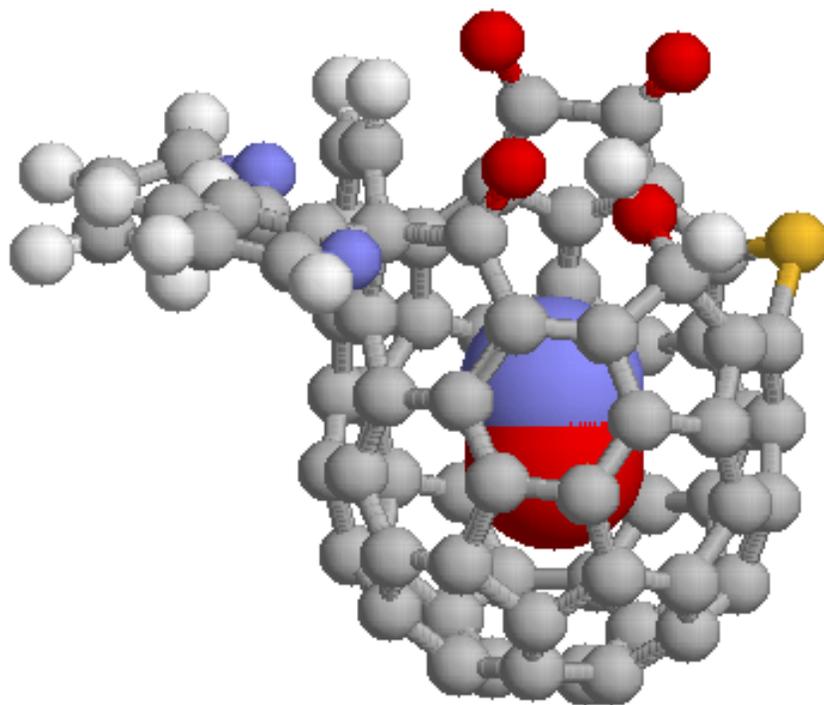


Fig. 1.