

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

Anonymous Referee #2

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This paper describes an interesting approach to the study of paramagnetic NO molecules encapsulated in open-cage C60 fullerenes by pulse EPR methods, from echo-detected, field-swept EPR to nutation and ENDOR experiments. The overall data analysis of g-tensor and hyperfine/quadrupolar couplings is very thorough, presented very clearly and in all depth required. The experimental work is cleverly planned and nicely performed and analyzed. I only have a few comments and points that I would raise: A) The abstract needs some re-writing, compared to the clarity of the paper itself the abstract seems confusing, at least to me. B) At the end of the introduction, the authors state that a smaller g₃-value "deduced by an analysis of a CW measurement, necessitated confirmation by pulse ESR experiments, better suited for the study of very broad spectra." I would challenge this view of the difference in CW EPR and

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pulse EPR data content. In the case described here, the g_3 value of ~ 0.2 (instead of ~ 0.7 reported now in this paper) was deduced by fitting CW EPR spectra (if I understood correctly). In a way, ESE-detected EPR has a built in T2-filter that simplifies the spectra (reducing the broadness of the high-field region). I think the authors should point that out, as this is the real original point they have made here (or, if they think this is wrong, explain, why pulse EPR may be better suited). C) Figure 1 clearly needs to be amended with a chemical structure of the cage molecules - the DFT structures should also be shown from a side view, not only the top view. D) Figure 4 (PEANUT): the authors should explain the three black lines in the graph E) last line on page 6: "level splitting" instead of "spitting" F) Figs. 5 and 6 should be combined in one figure as a) and b) or Fig 6 should be moved into the SI G) Again Figs 7 and 8 should be combined into one figure as a) and b) H) Page 10, beginning of 3.2: Would the authors expect a better resolution at intermediate field values when the frequencies for the ENDOR experiments are varied (through changes in g -strain?)? I) Figures 9, 10, 11: While I am usually all for original presentation of data, in this case I just think that plotting the three spectra in three rows above each other in Fig. 9 (without additional 3-D shift) would make it easier to see the "evolution" of orientation-dependent spectra. Then, Figs. 10 (and 11, I believe) could also be included in this figure.

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