Dear Editor,

Thank you for the review of our manuscript "**The role of molecular properties of mononitrofluoranthenes to their mutagenic activity: insight from *ab initio* and DFT calculations**" (Manuscript number 8173-45275-2-CE; https://doi.org/10.2298/JSC190509045O) prepared for the special issue of the Journal of the Serbian Chemical Society devoted to 70th birthday of Academician Prof. Emeritus Miljenko Perić.

We have corrected our manuscript according to the comments of the reviewer and the journal manager. We are sending the explanations about how the reviewer's comments have been incorporated. The answers to the queries of the journal manager are indicated within the text. The corrections to the manuscript are highlighted in yellow.

Wit best regards,

Bojana Ostojić

Response to the comments of the reviewer:

line 34 NF is not defined previously (only in the abstract, but not in the main text).
Response: We have added the abbreviation NFs in the main text.

line 53 and line 54 references for B3LYP and cam-B3LYP are missing
Response: We have added the references for these two functionals.

line 71 10-14 a.u - -14 a.u should bin in superscript
Response: We have corrected the superscript.

line 73 Werner et al., 2008 is not necessary - it is already given as reference.

Response: We have removed the part of the text.

Taaable I - FLU should be defined in the caption of the table
Response:

We have added explanation for fluoranthene in the caption of the table.

Table II - level of theory for geometries should be indicated (in the text it is written B3LYP/6-311+G(2df,p))
Response: We have added in Table II the level of theory used for the optimized

structures.

line 161 "Different regions ranging from positive (blue) to negative (red) electrostatic potentials" - green colour should be added (neutral?)
Response: We have added in the text the explanation about the colours employed for the MESP surfaces.

Figure 3 - Colour range (with values, max-min) should be indicated (blue-green-red)
Response: We have made a new Figure 3 with the colour mapping toolbar.

Figure 7 and Figure 8 - vector displacements are hard to see - if possible they should be redrawn
Response: We have made new figures 7 and 8 so that the displacements vectors are redrawn.

REPORT:
This is an interesting and original contribution to the development of relationship between molecular properties and experimental mutagenic activities of mononitrofluroanthenes. The structures, stabilities, ionization potentials and electron affinities, NICS indexes, dipole moments, hyper-polarizabilities, vibrational spectra, molecular electrostatic potential, etc. of 5 mononitrofluroanthenes were calculated. The paper is well written, and presented, the calculations have been carried out properly, and conclusions seems adequate. Consequently, I suggest to accept it for publication as is. Minor, technical details are given in "Additional Comments"

In my opinion, this manuscript should:
be published as is

If manuscript is suitable for publishing, referees recommendation :
Original scientific paper