Belgrade, May 21th 2019

Dear prof. Juranić,

Authors are grateful for the comments from the reviewer. They are followed and corrections are made as requested. These improvements significantly added to the quality of work and therefore we hope that our article now fulfils the requirements of the journal.

The answers to the comments of authors are written point-by-point and changes are clearly marked by the bold text in answer.

**Referee: 1**

**Q1:** Line 159: "DPPH•7,16." In pdf version of text the number 16 is
strikethrough, please check the written number.

**A1:** In the revisited version of Manuscript this is corrected and number 16 is deleted.

**Q2:** Table 2: The enumeration of atoms is not as in Fig 2.; N11
instead of N1, C21 instead of C2, .... As well as in line 190: "especially
on N13 and N14,"; and line 193: "N13 and N14 atoms". Enumeration must be
aligned in Fig 2 and Table 2 as well as in the text.

**A2:** Enumeration in Table 2 and text of Manuscript is aligned with enumeration in Figure 2.

*This induces more noticeable changes in charge on nitrogen and sulfur atoms, with a decrease in negative charge on nitrogen atoms, especially on* ***N2*** *and* ***N3****, and an increase in positive charge on sulfur atoms. The consequence of this is spin density delocalization though nitrogen and sulfur atoms. It should be noted that most of spin density is found localized on* ***N2*** *and* ***N3*** *atoms.*

**Q3:** Line 176 and 181. Clarify too which type of charge and spin density belong
those that are presented in Table 2. NBO, Mullican, etc.

**A3:** The type of charge and spin density is added in text and title of Table 2:

*The values of* ***NBO*** *charge and spin density in the mentioned structures are presented in Table 2.*

*TABLE 2.* ***NBO*** *charge and spin density on atoms of interest in the optimized structure of H2ABTS, ABTS•+ and ABTS2-*

**Q4:** Line 188. "The radical anion is formed when one of the electrons is lost
from dianion," the electron may be "taken" from dianion by some oxidizing
agent not just "lost". Please correct this sentence.

**A4:** The sentence is corrected as follows:

*The radical anion is formed when one of the electrons is* ***removed*** *from dianion, ABTS2-,* ***by oxidizing agent, in this case potassium persulfate.***