



№4 SDI Review Form 1.6

Journal Name:	American Chemical Science Journal
Manuscript Number:	Ms_ACSJ_22405
Title of the Manuscript:	Papaverin. Geometrical and Electronic Structure. Acidic Force.
Type of the Article	Original Research Papers

General guideline for Peer Review process:

This journal's peer review policy states that **NO** manuscript should be rejected only on the basis of '**lack of Novelty**', provided the manuscript is scientifically robust and technically sound.

To know the complete guideline for Peer Review process, reviewers are requested to visit this link:

(<http://www.sciencedomain.org/page.php?id=sdi-general-editorial-policy#Peer-Review-Guideline>)



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PART 1: Review Comments

	Reviewer's comment	Author's comment (if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
<u>Compulsory</u> REVISION comments	At the conclusion or in the abstract should specify who can use the results of this work and to whom they are useful.	The last sentence in the manuscript " Finally, made quantum-chemical calculations can promote the elaborations of new, more effective spasmolythics " is answered this remark. So the results can be more useful for chemists – synthetics, who synthesize spasmolythics.
<u>Minor</u> REVISION comments	✓ Tables 2-3 in the names of the columns should specify the unit of parameters ✓ Authors should indicate or formulate the criteria of geometric optimization of the computational process.	In tables 2-3 the unit of parameters indicated in the columns, 2 column – bond length in angstroms (Å), angles in degree, charges on the atoms in the size less value. Under finding minimum of molecular energy of system criteria is the precision of gradient method.
<u>Optional/General</u> comments	✓ It would be useful to specify the strategy choosing the step length optimization method and time of calculation.	For optimization of geometric structure of papaverine was chosen classic gradient method. As far as for us is known, applicable at the present time the methods of optimization are not really affected on qualitative results of quantum-chemical calculations. When choosing an optimization strategy between the time of calculation and step length preference for the accuracy of length