



SDI Review Form 1.6

Journal Name:	<u>British Journal of Applied Science & Technology</u>
Manuscript Number:	Ms_BJAST_33643
Title of the Manuscript:	Supersalts Na₂AlX₅ (X = F, Cl): quantum chemical study of the structure, vibration spectra and thermodynamic properties
Type of the Article	Original Research Article

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)
Compulsory REVISION comments		
Minor REVISION comments	The article is about theoretical investigation, prediction and design of novel supersalts Na_2AlX_5 ($\text{X} = \text{F}, \text{Cl}$). The methods section provides sufficient information. I only have some suggestions: In introduction please give knowledge about molecular orbitals Why is only AlF_4 and AlCl_4 were chosen. Are there two confirmation for Na_2AlX_5 In method part, calculation detail should be given References should be rewritten	▪ Only AlF_4 and AlCl_4 were chosen because: ✓ The molecules AlF_4 and AlCl_4 are the building blocks of the super salts considered. ✓ F and Cl. have high Electronegativity, smaller in size and reactivity. ✓ We were limited by our objectives and scope of the study even though it was interesting to involve Br and I too. ▪ Are there two conformations for Na_2AlX_5? : Yes, there are two conformers which correspond to the minimum of energy (two-cycled structure of C_{2v} symmetry and compact structure of C_s symmetry) were obtained. ▪ References in methodology/ Computation details part: The references were given in this part and found in the list.
Optional/General comments		