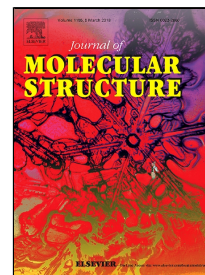


Accepted Manuscript



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PII: S0022-2860(18)30184-4
DOI: 10.1016/j.molstruc.2018.02.038
Reference: MOLSTR 24860
To appear in: *Journal of Molecular Structure*
Received Date: 15 December 2017
Revised Date: 06 February 2018
Accepted Date: 08 February 2018

Please cite this article as: I. Bayar, L. Khedhiri, S. Soudani, F. Lefebvre, V. Ferretti, C. Ben Nasr, Crystal structure, quantum mechanical investigation, IR and NMR spectroscopy of two new organic perchlorates: $(C_6H_{18}N_3) \cdot (ClO_4)_3 \cdot H_2O$ (I) and $(C_9H_{11}N_2) \cdot ClO_4$ (II), *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.02.038

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**Crystal structure, quantum mechanical investigation, IR and
NMR spectroscopy of two new organic perchlorates:
(C₆H₁₈N₃)·(ClO₄)₃·H₂O (I) and (C₉H₁₁N₂)·ClO₄(II)**

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Abstract

The reaction of perchloric acid with 1-(2-aminoethyl)piperazine or 5,6-dimethyl-benzimidazole results in the formation of 1-(2-aminoethyl)piperazine-1,4-dium triperchlorate hydrate (C₆H₁₈N₃)·(ClO₄)₃·H₂O (**I**) or 5,6-dimethyl-benzylimidazolium perchlorate (C₉H₁₁N₂)·ClO₄ (**II**). Both compounds were fully structurally characterized including single crystal X-ray diffraction analysis. Compound (**I**) crystallizes in the centrosymmetric triclinic space group $P\bar{1}$ with the lattice parameters $a = 7.455(2)$, $b = 10.462(2)$, $c = 10.824(2)$ Å, $\alpha = 80.832(2)$, $\beta = 88.243(2)$, $\gamma = 88.160(2)$ °, $Z = 2$ and $V = 832.77(3)$ Å³. Compound (**II**) has been found to belong to the $P2_1/c$ space group of the monoclinic system, with $a = 7.590(3)$, $b = 9.266(3)$, $c = 16.503(6)$ Å, $\beta = 107.38(2)$ °, $V = 1107.69(7)$ Å³ and $Z = 4$. The structures of (**I**) and (**II**) consist of slightly distorted [ClO₄]⁻ tetrahedra anions and 1-(2-aminoethyl)piperazine-1,4-dium trication (**I**) or 5,6-dimethyl-benzylimidazolium cations (**II**) and additionally a lattice water in (**I**). The crystal structures of

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