Title

Two three-electron bonds in two triatomic molecules? The cases of C2O and N2C in their ground states

Abstract

The chemical bonding of (Formula presented.) C (Formula presented.) O and (Formula presented.) N (Formula presented.) C is analyzed in this work through the topological quantum approach using the electronic localization function (ELF) at the CASSCF level and by energetic calculations at the CCSD(T) level using four different basis sets. The results show that the dissociation of the molecules occurs via cleavage of the C-C bond in the case of (Formula presented.) C (Formula presented.) O, while in the case of (Formula presented.) N (Formula presented.) C, it occurs via cleavage of the N-C bond. Furthermore, the results obtained with ELF show monosynaptic basins containing excess electrons and disynaptic basins with a low electron population. This leads us to indicate the existence of three-center-two-electron bonds according to previous results. From the valence bond model, a series of resonance structures have been proposed that support our calculations. In addition, the proposed structures have an ionic nature, indicating a charge shift character.

Authors

Pino-Rios R.; Denis-Alpizar O.

Author full names

Pino-Rios, Ricardo (56951201800); Denis-Alpizar, Otoniel (55546096800)

Author(s) ID

56951201800; 55546096800

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Affiliations

Química y Farmacia, Facultad de Ciencias de la Salud, Universidad Arturo Prat, Iquique, Chile; Instituto de Estudios de la Salud, Universidad Arturo Prat, Iquique, Chile; Grupo de Investigación en Física Aplicada, Instituto de Ciencias Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile, Santiago, Chile

Authors with affiliations

Pino-Rios R., Química y Farmacia, Facultad de Ciencias de la Salud, Universidad Arturo Prat, Iquique, Chile, Instituto de Estudios de la Salud, Universidad Arturo Prat, Iquique, Chile; Denis-Alpizar O., Grupo de Investigación en Física Aplicada, Instituto de Ciencias Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile, Santiago, Chile

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Correspondence Address

R. Pino-Rios; Facultad de Ciencias de la Salud, Universidad Arturo Prat, Iquique, 1100000, Chile; email: rpinorios@unap.cl; O. Denis-Alpizar; Grupo de Investigación en Física Aplicada, Instituto de Ciencias Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile, Santiago, Chile; email: otoniel.denis@uautonoma.cl

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