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The Bond Order Calculator: Updates

14 *Thursday Nov 2019*

Posted by egarcia in calculators, chemistry, minerazzi

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Tags
Bond Order, *bond order calculator*, *chemistry tools*, *tools*

New content was added to the bond order calculator page discussed at

https://irthoughts.wordpress.com/2018/12/20/bond-order-calculator-tool/

and available at

http://www.minerazzi.com/tools/bond-order/calculator.php

Enjoy it.

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Bond Order Calculator Tool

20 *Thursday Dec 2018*

Posted by egarcia in Algorithms, calculators, chemical mining, chemistry, Chemometrics, Data Mining, Programming, Software

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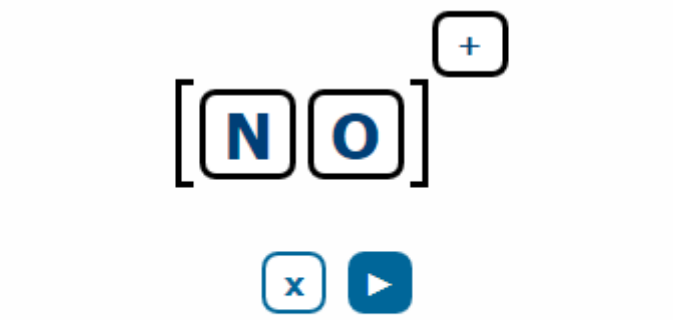
Tags

Bond Order, chemistry, Chemistry Calculator, chemistry tools, Diatomic Species



Unique Elements:	$_{7}$N, $_{8}$O
Total number of electrons, n:	14
antibonding electrons, na:	4
bonding electrons, nb:	10
electrons ratio, na/nb:	0.40
electrons product, 2nanb:	80
Bond Order, BO:	3.00

This tool computes bond orders of diatomic species having up to 20 electrons, without using Molecular Orbital Theory! It is available at

http://www.minerazzi.com/tools/bond-order/calculator.php

We developed the tool inspired in Dr. Arijit Das set of innovative and time economic formulae for chemical education. His methodologies are suitable for computer-based learning (CBL) activities or for writing computer programs for solving chemistry problems.

Unlike with other bond order calculators, to use ours you don't need to write Lewis structures, and electron configurations, or count electrons, bonds, orbitals, and atoms. Just enter a chemical formula and the tool will do the rest for you.

In my opinion, students who know how to write programs for solving chemistry problems have an edge when taking quantitative courses like analytical chemistry, instrumental analysis, chemometrics, computational chemistry, and similar courses. I think they might be better prepared for multidisciplinary research work than those who cannot code.

Developing this tool was really gratifying as the work inspired us to derive an algorithm for predicting number of unpaired electrons and magnetic properties of single atoms, diatomic species, and their ions. Hopefully, this algorithm will be available early next year in the form of a new chemistry calculator.

We are also developing a tool that computes bond orders of all kind of species, including the polyatomic cases.

We are sincerely in debt to Dr. Arijit Das from Ramthakur College, Agartala, West Tripura, India for encouraging us to develop this tool for educators, scholars, and chemistry students.

Note:

This tool, as our Hydrocarbons Parser (http://www.minerazzi.com/tools/hydrocarbons/parser.php) is listed in the City College Chemistry Web Resources Guide at CUNY. Find them both in the guide Computational Chemistry category (https://library.ccny.cuny.edu/chemistry/computational)