Attachment 2: Software input & outputs

List of Contents:

General information about the computer software program

This program (BondLengthCalcV1) calculates chemical bond lengths using the potential wells of nuclei. It was written by Dariush H. Zadeh, PhD, PE in March 2021 to accompany a submitted article. The program needs an "input" file as shown in the submitted attachment/sample data. The atomic numbers of atoms as well as their symbols need to be provided in the input file. The article and this program were submitted in the honor of Prof. Peter Politzer. The program is a small gift to all researchers. The program can provide bond lengths between any two elements in the periodic Table up to the element "Hassium" or "Uno" with the atomic number of 108. Data is not available after Hassium.

The program needs an “input” file prepared in “**Notepad**”. The program provides an “output” file with all of the calculated data. You may change the name of “Sample input” to just “input” and run the program with it.

The “input” files need to have only 4 lines. Atomic symbol of first atom will be given on the first line. Atomic number of first atom will be given in the second line as a whole number with no decimal points. Atomic symbol of second atom will be given on the third line. Atomic number of second atom will be given in the fourth line as a whole number with no decimal points.

Once the “input” file becomes ready, you should click on the “BondLengthCalcV1” executable file to launch the computation. The output will be stored in the “output” file.

Sample "input" file for C-C bond

C Atomic Symbol of First Atom
6 Atomic Number of First Atom (whole number, no decimal point)
C Atomic Symbol of Second Atom
6 Atomic Number of Second Atom (whole number, no decimal point)

Sample "output" file for C-C bond

==========
Start of Input Data
==========
Symbol of First Atom C
Atomic Number of First Atom = 6

Symbol of Second Atom C
Atomic Number of Second Atom = 6
==========
End of Input Data
==========

Capacity of the last electronic shell of elements

Capacity of S shells are 2, (SP) shells 8, d shells 10 and f shells 14

Atom #	Symbol	Atomic NO	Capacity of the last electronic shell	Number of electrons in the last shell
1	C	6	8	4
2	C	6	8	4

==========
Data of the first atom
==========
Atomic Number= 6
Atomic Symbol= C

Electron Number	Ionization Energy (eV)	Apparant Nuclear Charge (ANC)	Electron Shieling Effect (ESE)	Bohr Radius, A	Distance to Well, A	Depth of Well, eV
1	11.2603	0.9099	-0.9099	0.5816	0.4071	-0.574
2	24.3845	1.3389	-0.4291	0.3952	0.2767	-0.398

3	47.8878	1.8764	-0.5374	0.2820	0.1974	-0.699
4	64.4935	2.1775	-0.3012	0.2430	0.1701	-0.455
5	392.0905	5.3690	-3.1915	0.0986	0.0690	-11.880
6	489.9932	6.0020	-0.6330	0.0882	0.0617	-2.634

Electron number 1 (e1) is the furthest away electron from nucleus

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==========
Data of the second atom
==========
Atomic Number= 6
Atomic Symbol= C

Electron Number	Ionization Energy (eV)	Apparant Nuclear Charge (ANC)	Electron Shieling Effect (ESE)	Bohr Radius, A	Distance to Well, A	Depth of Well, eV
1	11.2603	0.9099	-0.9099	0.5816	0.4071	-0.574
2	24.3845	1.3389	-0.4291	0.3952	0.2767	-0.398
3	47.8878	1.8764	-0.5374	0.2820	0.1974	-0.699
4	64.4935	2.1775	-0.3012	0.2430	0.1701	-0.455
5	392.0905	5.3690	-3.1915	0.0986	0.0690	-11.880
6	489.9932	6.0020	-0.6330	0.0882	0.0617	-2.634

Electron number 1 (e1) is the furthest away electron from nucleus

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==========
Single bond calculations
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First Approach (3rd order equation curve fitting)

Bond Index (BI) = 0.405990
Bond Length, A = 1.52227

Formulas which were used for this part of calculations:

Bond Index (BI) ={[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD21]}
WD21 means the first well distance of atom number 2 from nucleus
Bond Length, A = 0.6862*(BI^3)-2.6282*(BI^2)+3.9581*BI+0.3026

Second Approach (second order equation curve fitting)

Bond Index (BI) = 0.405990
Bond Length, A = 1.50549

Formulas which were used for this part of calculations:

Bond Index (BI) ={[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD21]}
WD21 means the first well distance of atom number 2 from nucleus
Bond Length, A = -0.8192*(BI^2)+2.5942*BI+0.5873

==========
Double bond calculations
==========

First Approach (3rd order equation curve fitting)

Bond Index (BI) = 0.313139
Bond Length, A = 1.30540

Formulas which were used for this part of calculations:

Bond Index (BI) =
{[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD12*WD21*WD22]^0.471}
WD12 means the second well distance of atom number 1 from nucleus
Bond Length, A = 0.6862*(BI^3)-2.6282*(BI^2)+3.9581*BI+0.3026

Second Approach (second order equation curve fitting)

Bond Index (BI) = 0.301070
Bond Length, A = 1.29408

Formulas which were used for this part of calculations:

Bond Index (BI) =
{[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD12*WD21*WD22]^0.48}
WD12 means the second well distance of atom number 1 from nucleus
Bond Length, A = -0.8192*(BI^2)+2.5942*BI+0.5873

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Triple bond calculations

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First Approach (3rd order equation curve fitting)

Bond Index (BI) = 0.255398

Bond Length, A = 1.15349

Formulas which were used for this part of calculations:

Bond Index (BI) =
{[(Atomic Number 1).(Atomic Number2)]^0.25}*{[WD11*WD12*WD13*WD21*WD22*WD23]^0.297}

WD12 means the second well distance of atom number 1 from nucleus

Bond Length, A = 0.6862*(BI^3)-2.6282*(BI^2)+3.9581*BI+0.3026

Second Approach (second order equation curve fitting)

Bond Index (BI) = 0.240309

Bond Length, A = 1.16340

Formulas which were used for this part of calculations:

Bond Index (BI) =
{[(Atomic Number 1).(Atomic Number2)]^0.25}*{[WD11*WD12*WD13*WD21*WD22*WD23]^0.305}

WD12 means the second well distance of atom number 1 from nucleus

Bond Length, A = -0.8192*(BI^2)+2.5942*BI+0.5873

Sample "input" file for H-Cl bond

H	Atomic Symbol of First Atom
1	Atomic Number of First Atom (whole number, no decimal point)
Cl	Atomic Symbol of Second Atom
17	Atomic Number of Second Atom (whole number, no decimal point)

Sample "output" file for H-Cl bond

==========

Start of Input Data

==========

Symbol of First Atom H
Atomic Number of First Atom = 1

Symbol of Second Atom Cl
Atomic Number of Second Atom = 17

==========

End of Input Data

==========

Capacity of the last electronic shell of elements

Capacities of S shells are 2, (SP) shells 8, d shells 10 and f shells 14

Atom #	Symbol	Atomic NO	Capacity of the last electronic shell	Number of electrons in the last shell
1	H	1	2	1
2	Cl	17	8	7

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Data of the first atom

==========

Atomic Number= 1
Atomic Symbol= H

Electron Number	Ionization Energy (eV)	Apparant Nuclear Charge (ANC)	Electron Shieling Effect (ESE)	Bohr Radius, A	Distance to Well, A	Depth of Well, eV
1	13.5984	0.9999	-0.9999	0.5292	0.3705	-0.693

Electron number 1 (e1) is the furthest away electron from nucleus

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==========
Data of the second atom
==========
Atomic Number= 17
Atomic Symbol= Cl

Electron Number	Ionization Energy (eV)	Apparant Nuclear Charge (ANC)	Electron Shieling Effect (ESE)	Bohr Radius, A	Distance to Well, A	Depth of Well, eV
1	12.9676	0.9764	-0.9764	0.5420	0.3794	-0.661
2	23.8136	1.3232	-0.3468	0.3999	0.2800	-0.318
3	39.8000	1.7106	-0.3874	0.3094	0.2165	-0.459
4	53.2400	1.9784	-0.2679	0.2675	0.1872	-0.367
5	67.6800	2.2307	-0.2522	0.2372	0.1661	-0.390
6	96.9400	2.6697	-0.4390	0.1982	0.1388	-0.813
7	114.2013	2.8976	-0.2280	0.1826	0.1278	-0.458

Electron number 1 (e1) is the furthest away electron from nucleus

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==========
Single bond calculations
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First Approach (3rd order equation curve fitting)

Bond Index (BI) = 0.285383
Bond Length, A = 1.23407

Formulas which were used for this part of calculations:

Bond Index (BI) ={[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD21]}
WD21 means the first well distance of atom number 2 from nucleus
Bond Length, A = 0.6862*(BI^3)-2.6282*(BI^2)+3.9581*BI+0.3026

Second Approach (second order equation curve fitting)

Bond Index (BI) = 0.285383
Bond Length, A = 1.26092

Attachment 2: Software input & outputs

Molecular theory considering nuclear potential wells, by Dariush Habibollah Zadeh, March 2021

Formulas which were used for this part of calculations:

Bond Index (BI) ={[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD21]}

WD21 means the first well distance of atom number 2 from nucleus

Bond Length, A = -0.8192*(BI^2)+2.5942*BI+0.5873

Multiple bonds are not possible due to electronic structures of atoms

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Sample "input" file for C-N bond

C	Atomic Symbol of First Atom
6	Atomic Number of First Atom (whole number, no decimal point)
N	Atomic Symbol of Second Atom
7	Atomic Number of Second Atom (whole number, no decimal point)

Sample "output" file for C-N bond

==========

Start of Input Data

==========

Symbol of First Atom C
Atomic Number of First Atom = 6

Symbol of Second Atom N
Atomic Number of Second Atom = 7

==========

End of Input Data

==========

Capacity of the last electronic shell of elements

Capacities of S shells are 2, (SP) shells 8, d shells 10 and f shells 14

Atom #	Symbol	Atomic NO	Capacity of the last electronic shell	Number of electrons in the last shell
1	C	6	8	4
2	N	7	8	5

==========

Data of the first atom

==========

Atomic Number= 6
Atomic Symbol= C

Electron Number	Ionization Energy (eV)	Apparant Nuclear Charge (ANC)	Electron Shieling Effect (ESE)	Bohr Radius, A	Distance to Well, A	Depth of Well, eV
1	11.2603	0.9099	-0.9099	0.5816	0.4071	-0.574
2	24.3845	1.3389	-0.4291	0.3952	0.2767	-0.398

3	47.8878	1.8764	-0.5374	0.2820	0.1974	-0.699
4	64.4935	2.1775	-0.3012	0.2430	0.1701	-0.455
5	392.0905	5.3690	-3.1915	0.0986	0.0690	-11.880
6	489.9932	6.0020	-0.6330	0.0882	0.0617	-2.634

Electron number 1 (e1) is the furthest away electron from nucleus

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==========
Data of the second atom
==========
Atomic Number= 7
Atomic Symbol= N

Electron Number	Ionization Energy (eV)	Apparant Nuclear Charge (ANC)	Electron Shieling Effect (ESE)	Bohr Radius, A	Distance to Well, A	Depth of Well, eV
1	14.5341	1.0337	-1.0337	0.5119	0.3583	-0.741
2	29.6012	1.4752	-0.4415	0.3587	0.2511	-0.452
3	47.4453	1.8677	-0.3924	0.2833	0.1983	-0.508
4	77.4735	2.3866	-0.5189	0.2217	0.1552	-0.859
5	97.8901	2.6827	-0.2961	0.1973	0.1381	-0.551
6	552.0673	6.3709	-3.6882	0.0831	0.0581	-16.291
7	667.0461	7.0030	-0.6321	0.0756	0.0529	-3.069

Electron number 1 (e1) is the furthest away electron from nucleus

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==========
Single bond calculations
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First Approach (3rd order equation curve fitting)

Bond Index (BI) = 0.371392
Bond Length, A = 1.44525

Formulas which were used for this part of calculations:

Bond Index (BI) ={[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD21]}
WD21 means the first well distance of atom number 2 from nucleus
Bond Length, A = 0.6862*(BI^3)-2.6282*(BI^2)+3.9581*BI+0.3026

Second Approach (second order equation curve fitting)

Bond Index (BI) = 0.371392
Bond Length, A = 1.43777

Formulas which were used for this part of calculations:

Bond Index (BI) ={[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD21]}
WD21 means the first well distance of atom number 2 from nucleus
Bond Length, A = -0.8192*(BI^2)+2.5942*BI+0.5873

==========
Double bond calculations
==========

First Approach (3rd order equation curve fitting)

Bond Index (BI) = 0.292781
Bond Length, A = 1.25339

Formulas which were used for this part of calculations:

Bond Index (BI) =
{[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD12*WD21*WD22]^0.471}
WD12 means the second well distance of atom number 1 from nucleus
Bond Length, A = 0.6862*(BI^3)-2.6282*(BI^2)+3.9581*BI+0.3026

Second Approach (second order equation curve fitting)

Bond Index (BI) = 0.280928
Bond Length, A = 1.25143

Formulas which were used for this part of calculations:

Bond Index (BI) =
{[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD12*WD21*WD22]^0.48}
WD12 means the second well distance of atom number 1 from nucleus
Bond Length, A = -0.8192*(BI^2)+2.5942*BI+0.5873

==========

Triple bond calculations

==========

First Approach (3rd order equation curve fitting)

Bond Index (BI) = 0.248651

Bond Length, A = 1.13484

Formulas which were used for this part of calculations:

Bond Index (BI) =
{[(Atomic Number 1).(Atomic Number2)]^0.25}*{[WD11*WD12*WD13*WD21*WD22*WD23]^0.297}

WD12 means the second well distance of atom number 1 from nucleus

Bond Length, A = 0.6862*(BI^3)-2.6282*(BI^2)+3.9581*BI+0.3026

Second Approach (second order equation curve fitting)

Bond Index (BI) = 0.233550

Bond Length, A = 1.14849

Formulas which were used for this part of calculations:

Bond Index (BI) =
{[(Atomic Number 1).(Atomic Number2)]^0.25}*{[WD11*WD12*WD13*WD21*WD22*WD23]^0.305}

WD12 means the second well distance of atom number 1 from nucleus

Bond Length, A = -0.8192*(BI^2)+2.5942*BI+0.5873

Sample "input" file for C-Pb bond

C	Atomic Symbol of First Atom
6	Atomic Number of First Atom (whole number, no decimal point)
Pb	Atomic Symbol of Second Atom
82	Atomic Number of Second Atom (whole number, no decimal point)

Sample "output" file for C-Pb bond

==========

Start of Input Data

==========

Symbol of First Atom C
Atomic Number of First Atom = 6

Symbol of Second Atom Pb
Atomic Number of Second Atom = 82

==========

End of Input Data

==========

Capacity of the last electronic shell of elements

Capacity of S shells are 2, (SP) shells 8, d shells 10 and f shells 14

Atom #	Symbol	Atomic NO	Capacity of the last electronic shell	Number of electrons in the last shell
1	C	6	8	4
2	Pb	82	8	4

==========

Data of the first atom

==========

Atomic Number= 6
Atomic Symbol= C

Electron Number	Ionization Energy (eV)	Apparant Nuclear Charge (ANC)	Electron Shieling Effect (ESE)	Bohr Radius, A	Distance to Well, A	Depth of Well, eV
1	11.2603	0.9099	-0.9099	0.5816	0.4071	-0.574
2	24.3845	1.3389	-0.4291	0.3952	0.2767	-0.398
3	47.8878	1.8764	-0.5374	0.2820	0.1974	-0.699

4	64.4935	2.1775	-0.3012	0.2430	0.1701	-0.455
5	392.0905	5.3690	-3.1915	0.0986	0.0690	-11.880
6	489.9932	6.0020	-0.6330	0.0882	0.0617	-2.634

Electron number 1 (e1) is the furthest away electron from nucleus

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==========
Data of the second atom
==========
Atomic Number= 82
Atomic Symbol= Pb

Electron Number	Ionization Energy (eV)	Apparant Nuclear Charge (ANC)	Electron Shieling Effect (ESE)	Bohr Radius, A	Distance to Well, A	Depth of Well, eV
1	7.4167	0.7384	-0.7384	0.7166	0.5016	-0.378
2	15.0325	1.0513	-0.3129	0.5034	0.3524	-0.228
3	31.9373	1.5323	-0.4810	0.3453	0.2417	-0.511
4	42.3326	1.7642	-0.2318	0.3000	0.2100	-0.284
5	68.8000	2.2490	-0.4849	0.2353	0.1647	-0.756
6	82.9000	2.4688	-0.2197	0.2143	0.1500	-0.376
7	100.1000	2.7128	-0.2440	0.1951	0.1365	-0.459

Electron number 1 (e1) is the furthest away electron from nucleus

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==========
Single bond calculations
==========

First Approach (3rd order equation curve fitting)

Bond Index (BI) = 0.961837
Bond Length, A = 2.28882

Formulas which were used for this part of calculations:

Bond Index (BI) ={[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD21]}
WD21 means the first well distance of atom number 2 from nucleus
Bond Length, A = 0.6862*(BI^3)-2.6282*(BI^2)+3.9581*BI+0.3026

Second Approach (second order equation curve fitting)

Bond Index (BI) = 0.961837
Bond Length, A = 2.32463

Formulas which were used for this part of calculations:

Bond Index (BI) ={[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD21]}
WD21 means the first well distance of atom number 2 from nucleus
Bond Length, A = -0.8192*(BI^2)+2.5942*BI+0.5873

==========
Double bond calculations
==========

First Approach (3rd order equation curve fitting)

Bond Index (BI) = 0.744446
Bond Length, A = 2.07575

Formulas which were used for this part of calculations:

Bond Index (BI) =
{[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD12*WD21*WD22]^0.471}
WD12 means the second well distance of atom number 1 from nucleus
Bond Length, A = 0.6862*(BI^3)-2.6282*(BI^2)+3.9581*BI+0.3026

Second Approach (second order equation curve fitting)

Bond Index (BI) = 0.718662
Bond Length, A = 2.02856

Formulas which were used for this part of calculations:

Bond Index (BI) =
{[(Atomic Number 1).(Atomic Number 2)]^0.25}*{[WD11*WD12*WD21*WD22]^0.48}
WD12 means the second well distance of atom number 1 from nucleus
Bond Length, A = -0.8192*(BI^2)+2.5942*BI+0.5873

==========
Triple bond calculations
==========

First Approach (3rd order equation curve fitting)

Bond Index (BI) = 0.596190
Bond Length, A = 1.87362

Formulas which were used for this part of calculations:

Bond Index (BI) =
{[(Atomic Number 1).(Atomic Number2)]^0.25}*{[WD11*WD12*WD13*WD21*WD22*WD23]^0.297}
WD12 means the second well distance of atom number 1 from nucleus
Bond Length, A = 0.6862*(BI^3)-2.6282*(BI^2)+3.9581*BI+0.3026

Second Approach (second order equation curve fitting)

Bond Index (BI) = 0.563906
Bond Length, A = 1.78969

Formulas which were used for this part of calculations:

Bond Index (BI) =
{[(Atomic Number 1).(Atomic Number2)]^0.25}*{[WD11*WD12*WD13*WD21*WD22*WD23]^0.305}
WD12 means the second well distance of atom number 1 from nucleus
Bond Length, A = -0.8192*(BI^2)+2.5942*BI+0.5873
