AOMix 6.52 x86

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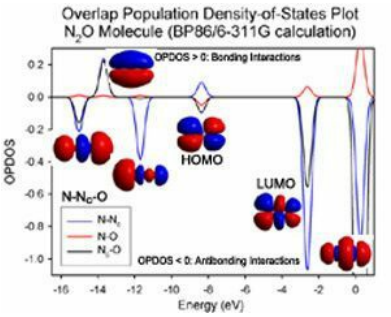


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AOMix Revision 6.52 (Copyright: S.I. Gorelsky, 2003-2011)
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**********************************************************************
Use of the AOMix program should be acknowledged in publications as:
  S. I. Gorelsky, AOMix program, http://www.sg-chem.net/
**********************************************************************
Spin-unrestricted calculation,  MPA

Molecule:    CH(4)
Details:#P B3LYP/TZVP SCF=Tight Pop=Full IOp(3/33=1) NoSymm
Source file:.\FRAGM2.LOG
  25 orbitals(   25 canonical)    5 alpha +   2 beta electrons
Created Thu Jun  1 19:29:07 2017 from Gaussian
Every atom is a fragment. Number of atoms:   2

The largest LCAO coefficient for alpha-spin MOs is     4.572

The largest LCAO coefficient for  beta-spin MOs is     4.604

The lowest eigenvalues of the overlap matrix:
-----------------------------------------------
 7.385876182965483E-003
 4.043372908053740E-002
 4.802766448738517E-002
 0.154259791682187
 0.161272894302842
 0.161272894302842


2-CENTER BOND ORDERS BETWEEN FRAGMENTS, B(AB) and its components,
2(PA*S)(PA*S) and 2(PB*S)(PB*S), and TOTAL OVERLAP POPULATIONS (TOPs)

                 Wiberg     Mayer bond orders(>0.01)  Overlap populations
  A     B    (P*S)(P*S)    B(AB)  B(alpha) B(beta)  TOP(alpha) TOP(beta)
----- ----- ----------   ------- -------- -------  ---------  ---------
  1C    2H     0.840      0.952   0.489   0.462       0.284     0.369


WIBERG BOND ORDERS BETWEEN FRAGMENTS IN THE LOWDIN BASIS
FRAG     1C
    -------
  2H   1.100

WIBERG BOND ORDERS BETWEEN FRAGMENTS IN THE LOWDIN BASIS, ALPHA-SPIN ORBITALS
FRAG     1C
```

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                    A O M i x 6.52

  This program calculates contributions of fragment orbitals, atoms,
  or groups of atoms to molecular orbitals and calculates electron
  populations of these fragments, overlap populations between them,
  2-, 3-, 4-, 5- and 6-center bond orders, and other MO descriptors.

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  Centre for Catalysis Research & Innovation, Department of Chemistry,
          University of Ottawa, http://www.sg-chem.net/aomix/

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 transmitted, or stored only in accord with that license. Please refer
 to the AOMix manual to details.
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 Enter the name of the output file to be processed and,if applicable,
 or the name of the user-defined fragment file; or the the FO keyword
 to generate a new wavefunction from the output files of
 molecular fragments; or the combination (a file name followed by
 the FO keyword) to perform AOMix-FO calculation:
```

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