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================================================================================
 /usr/local/Intel/compiler90/bin/ifc -O3
 Thu Oct  5 23:54:39 CEST 2006
 reinh@hydrogene
================================================================================


Started ICMP MOL;  date: 25.10.06 time: 19:21:02


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 I C M P  -  1 molecule; from 1D ring systems
 correlation by MP2 and others

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 MP2 PERTURBATION CORRECTIONS
 EPSTEIN-NESBET PERTURBATIONS

 third-order Moeller-Plesset perturbation theory via determinants


 third-order Epstein-Nesbet perturbation theory via determinants

 CI of SINGLES and DOUBLES
 READING UNFORMATTED INTEGRALS, MAX. BUFFER LENGTH         4096
 THRESHOLD FOR BIELECTRONIC INTEGRALS IS: 0.1000E-09
 THE PRINT LEVEL IS SET TO   0

 taking into account all possible determinants




 READ INFORMATION ON SYSTEM
        NATOMS            1
        NBAS              2


 READING VECTOR FROM UNIT          31
 READING OVERLAP MATRIX FROM UNIT          14


        NOCC              1
        NVIRT             1

 READING FOCK MATRIX FROM UNIT          23

        E0 E1 E2   0.000000000000000E+000  -3.88207578790000
  1.02691540590000

 TRANSFORMED FOCK MATRIX
 LARGEST ELEMENT BETWEEN OCC/VIRT: 0.174648E-06

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 ORBEN:            1 -0.914122487983658        participating
 ORBEN:            2   1.40061881408182        participating

 THE ABSOLUTE MAXIMUM NUMBER OF BIELECTRONIC INTEGRALS IS           6
         6
```



```
 WE READ THE INTEGRALS FROM FILE           53

 OPENED UNIT           56  AS FILE OOOO1
 OPENED UNIT           57  AS FILE OOOV1
 OPENED UNIT           58  AS FILE OVOV1
 OPENED UNIT           59  AS FILE OOVV1
 OPENED UNIT           60  AS FILE OVVV1
 OPENED UNIT           61  AS FILE VVVV1
 OPENED UNIT           62  AS FILE OOOO2
 OPENED UNIT           63  AS FILE OOOV2
 OPENED UNIT           64  AS FILE OVOV2
 OPENED UNIT           65  AS FILE OOVV2
 OPENED UNIT           66  AS FILE OVVV2
 OPENED UNIT           67  AS FILE VVVV2

 OPENED UNIT           53  FOR UNFORMATTED READING
 WE FOUND A BUFFER LENGTH OF         4096

 WE REACHED THE ONE-ELECTRON SECTION

 CLOSED UNIT           53


READ         6 INTEGRALS
KEPT         6 INTEGRALS (100.0%)


NUMBER OF INTEGRALS IN THE DIFFERENT CLASSES:
 TYPE         N1          N2
             (AABC)      (ABCD)
------------------------------
  OOOO           1           0
  OOOV           1           0
  OVOV           1           0
  OOVV           1           0
  OVVV           1           0
  VVVV           1           0
 ------------------------------

 ALL BIELECTRONIC INTEGRALS FIT INTO THE DEFINED BUFFER
 SEGMENT            1 : STARTING AT:           1  ENDING AT:           1
 SEGMENT            2 : STARTING AT:           2  ENDING AT:           2
 SEGMENT            3 : STARTING AT:           3  ENDING AT:           3
 SEGMENT            4 : STARTING AT:           4  ENDING AT:           4
 SEGMENT            5 : STARTING AT:           5  ENDING AT:           5
 SEGMENT            6 : STARTING AT:           6  ENDING AT:           6
 SEGMENT            7 : STARTING AT:           7  ENDING AT:           6
 SEGMENT            8 : STARTING AT:           7  ENDING AT:           6
 SEGMENT            9 : STARTING AT:           7  ENDING AT:           6
 SEGMENT           10 : STARTING AT:           7  ENDING AT:           6
 SEGMENT           11 : STARTING AT:           7  ENDING AT:           6
 SEGMENT           12 : STARTING AT:           7  ENDING AT:           6
 CHECKING ORDER OF INTEGRALS IN SEGMENT            1 ;           1  INTEGR
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT CHCK CPU      0.040
 INTEGRALS ARE WELL-ORDERED
 CHECKING ORDER OF INTEGRALS IN SEGMENT            2 ;           1  INTEGR
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT CHCK CPU      0.040
 INTEGRALS ARE WELL-ORDERED
 CHECKING ORDER OF INTEGRALS IN SEGMENT            3 ;           1  INTEGR
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT CHCK CPU      0.040
 INTEGRALS ARE WELL-ORDERED
```

```
 CHECKING ORDER OF INTEGRALS IN SEGMENT           4 ;           1  INTEGRALS
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT CHCK CPU      0.040
 INTEGRALS ARE WELL-ORDERED
 CHECKING ORDER OF INTEGRALS IN SEGMENT           5 ;           1  INTEGRALS
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT CHCK CPU      0.040
 INTEGRALS ARE WELL-ORDERED
 CHECKING ORDER OF INTEGRALS IN SEGMENT           6 ;           1  INTEGRALS
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT CHCK CPU      0.040
 INTEGRALS ARE WELL-ORDERED

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT R2I  CPU      0.040

 RECALCULATED ONE-ELECTRON ENERGY:  -3.88207578787797


 RECALCULATED TOTAL ENERGY          -2.85516038193657
 RECALCULATED ONE-ELECTRON ENERGY   -3.88207578787797
 RECALCULATED TWO-ELECTRON ENERGY    1.02691540594140
               NUCLEAR REPULSION   0.000000000000000E+000

 READ TOTAL ENERGY                  -2.85516038200000
 READ ONE-ELECTRON ENERGY           -3.88207578790000
 READ TWO-ELECTRON ENERGY            1.02691540590000
 READ NUCLEAR ENERGY                0.000000000000000E+000

   DIFFERENCES
  ONE EL. :   2.202948934382221E-011
  TWO EL. :   4.139977249906224E-011
  TOTAL   :   6.342926184288444E-011

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT ETOT CPU      0.040
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PREP CPU      0.040

 FOUND            3  PRIMARY DETERMINANTS FOR THE REFERENCE CELL


 GENERATED            4  SPIN DETERMINANTS
 THE DIMENSION OF THE HAMILTON MATRIX WILL BE            4  X            4

 THE REFERENCE IS AT POSITION            2
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MAKD CPU      0.040

  THE DIAGONAL OF THE HAMILTON MATRIX IS READY,
  AS WELL AS THE INTERACTIONS WITH THE REFERENCE,
             DIMENSION IS            4

  RECALCULATED MP2 - ENERGY      -0.011201774020

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT DETG CPU      0.040

 ---- MP2, again ... ----------



     CORRELATION ENERGY:      -0.011201774020

  CONTRIBUTIONS II -> KK      -0.011201774020
  CONTRIBUTIONS II -> KL       0.000000000000
  CONTRIBUTIONS IJ -> KK       0.000000000000
  CONTRIBUTIONS IJ -> KL       0.000000000000
                      ----------------------
            SUM               -0.011201774020
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  MP2L   - ENERGY :      -0.011201774020
  ==========================================


 -------- and spin-adapted Epstein-Nesbet ------

 ONE SECOND: we try the plain Epstein-Nesbet first


     CORRELATION ENERGY:      -0.015052083014

  CONTRIBUTIONS II -> KK      -0.015052083014
  CONTRIBUTIONS II -> KL       0.000000000000
  CONTRIBUTIONS IJ -> KK       0.000000000000
  CONTRIBUTIONS IJ -> KL       0.000000000000
                      ----------------------
            SUM               -0.015052083014


  EN 2   - ENERGY :      -0.015052083014
  ==========================================


 and our spin-adapted interaction-reduced Epstein-Nesbet


     CORRELATION ENERGY (SPIN-ADAPTED EPSTEIN-NESBET):
           total        -0.015052083014

  CONTRIBUTIONS II -> KK      -0.015052083014
  CONTRIBUTIONS II -> KL       0.000000000000
  CONTRIBUTIONS IJ -> KK       0.000000000000
  CONTRIBUTIONS IJ -> KL       0.000000000000
                      ----------------------
            SUM               -0.015052083014


  EN 2S  - ENERGY :      -0.015052083014
  ==========================================


TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PERT CPU      0.040

 Third-order Moeller-Plesset

  EHF    - ENERGY :      -2.855160381937
  ==========================================


  MP0    - ENERGY :      -1.828244975967
  ==========================================


  MP1    - ENERGY :      -1.026915405969
  ==========================================


  MP2S   - ENERGY :       0.000000000000
```

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  MP2T   - ENERGY :      -0.011201774020
  ============================================


  MP2    - ENERGY :      -0.011201774020
  ============================================


  SCSMP2 - ENERGY :      -0.013442128824
  ============================================


  A(3)   - ENERGY :      -0.005350189657
  ============================================


  B(3)   - ENERGY :       0.002484786163
  ============================================


  MP3    - ENERGY :      -0.002865403494
  ============================================


  MP2+3  - ENERGY :      -0.014067177514
  ============================================


TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MP3  CPU      0.040

 Third-order Epstein-Nesbet

  EHF    - ENERGY :      -2.855160381937
  ============================================


  EN0    - ENERGY :      -2.855160381937
  ============================================


  EN1    - ENERGY :       0.000000000000
  ============================================


  EN2    - ENERGY :      -0.015052083014
  ============================================


  EN3    - ENERGY :       0.000000000000
  ============================================


  E(2+3) - ENERGY :      -0.015052083014
  ============================================


TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT EN3  CPU      0.040

 spin-adapted EN3
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```
     CORRELATION ENERGY:      -0.015052083014

  CONTRIBUTIONS II -> KK      -0.015052083014
  CONTRIBUTIONS II -> KL       0.000000000000
  CONTRIBUTIONS IJ -> KK       0.000000000000
  CONTRIBUTIONS IJ -> KL       0.000000000000
                              ----------------------
            SUM               -0.015052083014

  EHF    - ENERGY :      -2.855160381937
  ============================================


  EN0    - ENERGY :      -2.855160381937
  ============================================


  EN1    - ENERGY :       0.000000000000
  ============================================


  EN2    - ENERGY :      -0.015052083014
  ============================================


  EN3    - ENERGY :       0.000000000000
  ============================================


  E(2+3) - ENERGY :      -0.015052083014
  ============================================


TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT EN3S CPU      0.040

 we try the CISD   via dressing of the CISD matrix


 R-R   R-S   R-D   S-S   S-D   D-D
  T     T     T     T     T     T

 THE MP2 - VECTOR has been recalculated

 WE FIND AS CORRELATION ENERGY :            -0.0112017740


         THE DAVIDSON PROCEDURE, taken from CASDI
       ---------------------------------------------

  ITER=  1  EIGENVALUE=  -0.014033221888, CONVERGENCE =  0.29D-01
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT IT 1 CPU      0.050
  ITER=  2  EIGENVALUE=  -0.014999848707, CONVERGENCE =  0.13D-02
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT IT 2 CPU      0.050
  ITER=  3  EIGENVALUE=  -0.015003474174, CONVERGENCE =  0.27D-16

 THE RESULT OF OUR EXERCISE AS normalized COEFFICIENTS:
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```
     2       0    0    0    0      0.997832368220
     3       1   -1    2   -2     -0.065741530722

 THE CI VECTOR IS ON FILE <CI_START>

 CONFIGURATION INTERACTION OF SINGLES AND DOUBLES:



    CORRELATION ENERGY:      -0.015003474537

  CONTRIBUTIONS II -> KK      -0.015003474900
  CONTRIBUTIONS II -> KL       0.000000000000
  CONTRIBUTIONS IJ -> KK       0.000000000000
  CONTRIBUTIONS IJ -> KL       0.000000000363
                             ---------------------
            SUM               -0.015003474537


  CISD   - ENERGY :      -0.015003474537
  ============================================



 AND ADDING THE DAVIDSON CORRECTION 1/c_0^2: (FACTOR  1.004349400293)
 (P.E.M.Siegbahn, Chem.Phys.Lett. 55 (1978) 386)

 ECORR:      -0.015068730654
  DAV-1  - ENERGY :      -0.015068730654
  ============================================




 OR THE CORRECTED CORRECTION c_0^2/(2c_0^2 - 1): (FACTOR  1.004368400214)
  (E.R.Davidson, D.W.Silver, Chem.Phys.Lett 52 (1977) 403)

 ECORR:      -0.015069015719
  DAV-2  - ENERGY :      -0.015069015719
  ============================================



TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT ICSD CPU      0.050

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT  ALL CPU      0.050

TOTAL CPUTIME:     0 hrs   0 mins and  0.0500 secs


Finished ICMP MOL;  date: 25.10.06 time: 19:21:02
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