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Jönsson, Per; Fischer, C. F

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MCHF calculations of isotope shifts;
I Program implementation and test runs
II Large-scale active space calculations

Per Jönsson
Department of Physics,
Lund Institute of Technology
P.O. Box 118, S-22100 Lund
Sweden
and
Charlotte Froese Fischer
Department of Computer Science,
Vanderbilt University
Box 1679 B, Nashville, TN 37235
USA
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Abstract

A new isotope shift program, part of the MCHF atomic structure package, has been written and tested. The program calculates the isotope shift of an atomic level from MCHF or CI wave functions. The program is specially designed to be used with very large CI expansions, for which angular data cannot be stored on disk. To explore the capacity of the program, large-scale isotope shift calculations have been performed for a number of low lying levels in \(B\ I\) and \(B\ II\). From the isotope shifts of these levels the transition isotope shift have been calculated for the resonance transitions in \(B\ I\) and \(B\ II\). The calculated transition isotope shifts in \(B\ I\) are in very good agreement with experimental shifts, and compare favourably with shifts obtained from a many-body perturbation calculation.
Part I
Isotope shift, program implementation and test runs

1 Introduction

The isotope shifts observed in atomic transitions arise from the finite nuclear mass and size. Conventionally the isotope shift is expressed as a sum of the mass and field shift. From a physical point of view the field shift is the more interesting, since it yields information about the nuclear charge distribution. One of the goals of ab initio calculations is to determine the mass shift as to enable the field shift to be extracted from the experimentally observed isotope shift. Unfortunately, it has shown exceedingly difficult to calculate the mass shift accurately. In order to obtain reliable results very large configuration expansions have to be used, where quadruple excitations are included.

The purpose of this study is to explore the capacity of a new isotope shift program, designed to be used with very large configuration interaction (CI) expansions.

2 Theory

The starting point for non-relativistic atomic calculations is the zero-order Hamiltonian (in a.u.)\(^1\)

\[
H_0 = \sum_{i=1}^{N} \left( -\frac{\nabla^2_i}{2m} - \frac{Z}{r_i} \right) + \sum_{i<j}^{N} \frac{1}{r_{ij}}
\]  

(1)

where the nucleus is assumed to be a point charge of infinite mass. In accurate calculations effects arising from the finite nuclear mass and size must be taken into account. This is normally done by treating these effects as perturbations.

2.1 Mass shift

For a finite nuclear mass, \(M\), the kinetic energy of the nucleus must be considered. Using the momentum conservation law in the center of mass coordinate system, the operator for the internal kinetic energy of an \(N\)-electron atom becomes [1]

\[
H_{\text{kin}} = -\sum_{i=1}^{N} \frac{\nabla^2_i}{2\mu} - \frac{1}{M} \sum_{i<j}^{N} \nabla_i \cdot \nabla_j.
\]

(2)

The first term includes a correction to the electron mass in which the mass \(m\) is replaced by the reduced mass, \(\mu = Mm/(M + m)\). This correction to the electron mass can be accounted for by multiplying the energy levels \(E_0\), calculated from the zero-order Hamiltonian, with \(M/(M + m)\). The resulting energy correction to the level \(E_0\) is then given by

\[
E_{\text{mass}} = -E_0 \frac{m}{M + m}
\]

(3)

\(^1\)In atomic units \(m = 1\), but it is included explicitly to avoid misinterpretations.
This is the normal mass shift (nms). The inclusion of the second term leads to an additional energy correction known as the specific mass shift (sms).

\[ E_{sms} = - \langle \psi | \frac{1}{M} \sum_{i<j}^{N} \nabla_i \cdot \nabla_j | \psi \rangle \]  \hspace{1cm} (4)

As first noted by Stone [2] the specific mass shift operator can be put into a more familiar tensorial form.

\[ H_{sms} = - \frac{1}{M} \sum_{i<j}^{N} \nabla_i \cdot \nabla_j = - \frac{1}{M} \sum_{i<j}^{N} \nabla^{(1)}_i \cdot \nabla^{(1)}_j \]  \hspace{1cm} (5)

where

\[ \nabla^{(1)} = C^{(1)} \frac{\partial}{\partial r} - \frac{\sqrt{2}}{r} (C^{(1)})^{(1)} \]  \hspace{1cm} (6)

Using the relation

\[ \langle l|| (C^{(1)})^{(1)} || l' \rangle = \frac{l(l+1) - 2 - l'(l'+1)}{2\sqrt{2}} \langle l|| C^{(1)} || l' \rangle \]  \hspace{1cm} (7)

it is seen that the gradient operator can be factorized in a radial and an angular part

\[ \nabla^{(1)} = \nabla_r C^{(1)} \]  \hspace{1cm} (8)

where the radial part is given by

\[ \nabla_r = \frac{\partial}{\partial r} - \frac{l(l+1) - 2 - l'(l'+1)}{2r} \]  \hspace{1cm} (9)

Finally, substituting this into eq.(5) we get the tensorial form of the specific mass shift operator

\[ H_{sms} = - \frac{1}{M} \sum_{i<j}^{N} \nabla_r \nabla_r (C^{(1)}_i \cdot C^{(1)}_j) \]  \hspace{1cm} (10)

This tensorial form is the same as that for the \( k = 1 \) term in the expression for the electrostatic interaction between the electrons

\[ \sum_{i<j}^{N} \frac{1}{r_{ij}} = \sum_{i<j}^{N} \sum_{k} \frac{r_{i}^{k}}{r_{i}^{k+1}} (C^{(k)}_i \cdot C^{(k)}_j) \]  \hspace{1cm} (11)

Thus, the computational apparatus set up for the calculation of the electrostatic interaction matrix elements can, with small modifications, be used also for the specific mass shift.

2.2 Field shift

Due to the finite size of the nucleus the potential inside the nuclear charge distribution deviates from the potential of a point charge \( Z \). For light atoms, where non-relativistic wavefunctions can be used, the resulting energy correction to the level \( E_0 \) is given by

\[ E_{fs} = \frac{2\pi}{3} Z \langle \psi_N^2 \rangle |\psi(0)|^2 \]  \hspace{1cm} (12)
where \( (r_N^2) \) is the mean square radius of the nucleus. Using the Dirac delta function the field shift \( (fs) \) can be written

\[
E_{fs} = \frac{2\pi}{3} Z(r_N^2) |\psi(0)|^2 = \frac{2\pi}{3} Z(r_N^2) \langle \psi | \sum_{i=1}^{N} \delta(r_i) |\psi \rangle
\]

(13)

Noting that \( 4\pi r^2 \delta(r) = \delta(r) \) we can write the field shift operator in tensorial form

\[
H_{fs} = \frac{1}{6} Z(r_N^2) \sum_{i=1}^{N} \delta(r_i) r_i^{-2}
\]

(14)

3 Program implementation

The present isotope shift program, part of the multi-configuration Hartree-Fock (MCHF) atomic structure package [3], is a complement to the old isotope shift program [4] that requires access to the angular files produced by the MCHF_NONH or MCHF_BREIT programs [5, 6]. The new program calculates the isotope shift without any reference to files containing angular information and can therefore be used with very large CI expansions.

3.1 Outline of method

In the multi-configuration Hartree-Fock method the atomic state wavefunction, \( \psi \), is expanded in terms of configuration-state functions (CSFs) with the same \( LS \) term

\[
\psi = \sum_{i=1}^{m} c_i \Phi(\gamma_i LS)
\]

(15)

The configuration-state functions, \( \Phi(\gamma_i LS) \), are antisymmetrized eigenfunctions to \( L^2, L_z, S^2, S_z \) and parity, which can be written as sums of products of spin-orbitals

\[
\phi(r, \theta, \varphi, \sigma) = \frac{1}{r} P_{nl}(r) Y_{lm}(\theta, \varphi) \xi_{m_s}(\sigma)
\]

(16)

where \( Y_{lm}(\theta, \varphi) \) is a spherical harmonic and \( \xi_{m_s}(\sigma) \) a spin function. By demanding the energy functional, \( \langle \psi \langle H_0 \rangle \psi \rangle \), for the atomic state wavefunction to be stationary with respect to variations in the radial functions and expansion coefficients, a system of coupled non-linear differential equations, one for each function, together with an eigenvalue problem for the expansion coefficients, is obtained. This problem is then solved by the self-consistent field (SCF) method [7, 8].

When a set of radial functions \( P_{nl}(r) \) has been obtained from an MCHF calculation, the atomic state wavefunction can be expanded in CSFs where now only the expansion coefficients have to be determined. This is done by diagonalizing the Hamiltonian matrix. Using a sparse matrix representation large expansions can be used. On a modern workstation expansions with more than 60 000 CSFs can be handled, the limit usually set by the available disk space. CI techniques also exist in which the explicit storage of the Hamiltonian matrix is avoided, and the eigenvectors obtained iteratively using Newton-Raphson type algorithms. For these techniques only the Hamiltonian matrix times a vector has to be stored, and therefore extremely large CI expansions can be used [9].
3.2 Calculation of the specific mass shift

Using standard Racah algebra techniques the evaluation of the specific mass shift from CSF expansions can be reduced to a summation over radial two-particle matrix elements.

\[
\langle \psi | H_{sms} | \psi \rangle = \sum_{i,i'} c_i c_{i'} \langle \gamma_i LS | H_{sms} | \gamma_{i'} LS \rangle
\]  

(17)

After the angular integrations have been performed, the matrix element between two configuration states may be expressed as

\[
\langle \gamma_i LS | H_{sms} | \gamma_{i'} LS \rangle = \sum_{n_l} \text{Coeff}(1, n_1 l_1, n_2 l_2; n_3 l_3, n_4 l_4) ii' \langle n_1 l_1 | \nabla_r | n_3 l_3 \rangle \langle n_2 l_2 | \nabla_r | n_4 l_4 \rangle
\]  

(18)

where the sum on \( n_l \) is over all ordered sets of four orbital indices, \( n_1 l_1, n_2 l_2; n_3 l_3, n_4 l_4, \) the first two from \( \gamma_i \) and the other two from \( \gamma_{i'} \). The coefficient \( \text{Coeff}(1, n_1 l_1, n_2 l_2; n_3 l_3, n_4 l_4) ii' \) is the same as the coefficient for the Slater integral \( R^1(n_1 l_1, n_2 l_2; n_3 l_3, n_4 l_4) \) in the expression for the electrostatic interaction between these two configuration states, is non-zero only if \( l_1 = l_3 \pm 1 \) and \( l_2 = l_4 \pm 1 \).

The radial matrix element of the field shift operator between one-electron orbitals is given by

\[
\langle n_l | \nabla_r | n_{l'} \rangle = \int_0^\infty P_{nl}(r) \left( \frac{d}{dr} \right) - \left( l(l+1) - l'(l'+1) \right) \frac{2}{r} P_{n'l'}(r) dr
\]  

(19)

3.3 Calculation of the field shift

In the same way the evaluation of the field shift operator from CSF expansions can be reduced to a summation over radial one-particle matrix elements.

\[
\langle \psi | H_{fs} | \psi \rangle = \sum_{i,i'} c_i c_{i'} \langle \gamma_i LS | H_{fs} | \gamma_{i'} LS \rangle
\]  

(20)

Since the field shift operator is a tensor operator of rank zero, the matrix element between two configuration states may be expressed as

\[
\langle \gamma_i LS | H_{fs} | \gamma_{i'} LS \rangle = \lambda \sum_{n_l} \text{Coeff}(1, n_1 l_1; n_2 l_2) ii' \langle n_1 l_1 | \delta(r) r^{-2} | n_2 l_2 \rangle
\]  

(21)

where the sum on \( n_l \) is over all ordered sets of two orbital indices, \( n_1 l_1; n_2 l_2, \) the first one from \( \gamma_i \) and the other one from \( \gamma_{i'} \). \( \lambda \) is a constant that contains the nuclear data and the coefficient \( \text{Coeff}(1, n_1 l_1; n_2 l_2) ii' \) is determined by standard Racah algebra techniques [10] and is nonzero only if \( l_1 = l_2 \).

The radial matrix element of the field shift operator between one-electron orbitals is given by

\[
\langle n_l | \delta(r) r^{-2} | n_{l'} \rangle = \delta_{l,0} \delta_{l',0} AZ(n_l) AZ(n_{l'})
\]  

(22)

where \( AZ(n_l) \) is the radial starting parameter

\[
AZ(n_l) = \left( \frac{P_{nl}(r)}{r_{l+1}} \right)_{r \to 0}
\]  

(23)
3.4 Program structure

Since the structure of the specific mass shift and field shift operators is very different, the former being a two-particle operator and the latter a one-particle operator, the calculation of the shifts is done by two different computer programs.

3.5 Specific mass shift program

This program calculates the specific mass shift parameter

\[ S = -\langle \psi | \sum_{i \neq j}^N \nabla_i \cdot \nabla_j | \psi \rangle \]  

(24)

From which the specific mass shift of a specific isotope with nuclear mass \( M \) is obtained by a scaling with \( 1/M \). The program is to a large extent based on the MCHF_NONH program for computing integrals of the non-relativistic Hamiltonian [5]. To run the program a number of input files have to be supplied. If the wavefunction has been obtained from an MCHF calculation the <name>.c and <name>.g files are read. The <name>.c file contains the configurations, their couplings and the weights. The <name>.g file contains the radial integrals (19). If, instead, the wavefunction has been obtained from a CI calculation the configuration weights are read from <name>.l. The <name>.g file must in this case be taken from the MCHF calculation that generated the orbital basis used in the CI calculation. The program operation can be summarized as follows:

- The configuration weights are read.
- The radial integrals are read and sorted according to the orbital ordering defined by the configuration list
- The program loops over the left- and right-hand configuration states and the weights \( c_i \) and \( c_{i'} \) are multiplied with the corresponding radial matrix elements and angular coefficients to give the contribution from the \( i, i' \) configuration pair. The contributions from each configuration pair are summed up to give the total value of the specific mass shift parameter.

Since the specific mass shift program only needs to evaluate the coefficients of the \( k = 1 \) term in the expression for the electrostatic interaction (11), the computation time can be cut down compared with the evaluation of the coefficients of all terms as done in MCHF_NONH. To restrict the evaluation to the \( k = 1 \) term changes have been made in the subroutine fano.

3.6 Field shift program

The expectation value of the field shift operator, a one-particle tensor operator of rank zero, is most easily computed within the framework of the previous hyperfine structure (hfs) program [11] based on Robb's program to evaluate reduced matrix elements of summations of one-particle tensor operators [10]. The calculation of the electron density at the nucleus \( |\psi(0)|^2 \) has been added as an option to the hfs program and from this quantity the field shift is easily obtained by multiplying with \( \frac{2e}{3}Z \langle r_N^2 \rangle \). The general structure of the program as well as the input files needed to run the program has been described in the original write-up of the hfs program [11].
4 Transition isotope shift

The observable effect of the isotope shift is a change of the transition energy between an upper and a lower atomic state. Different isotopes of a given element will have different transition energies. The measured difference in transition energy for two isotopes can directly be compared with the calculated difference.

4.1 Support program

Given the total non-relativistic energies $E_0$, the specific mass shift parameters $S$ and the electron densities $|\psi(0)|^2$ for the upper and lower atomic states as well as the nuclear masses $M$ and mean square radii $\langle r_N^2 \rangle$ for the isotopes, the transition energies of the isotopes can be calculated. These calculations are basically simple but involves a number of unit conversions. In order to minimize blunders a small support program has been written that calculates the transition energies from the parameters above. The program asks for the following data:

- specification of the transition
- zero order energy $E_0$ for the lower and upper state
- specific mass shift parameter $S$ for the lower and upper state
- electron density at the nucleus $|\psi(0)|^2$ for the upper and lower state
- number of isotopes
- isotope labels
- isotope masses $M$
- root mean square nuclear radii $\langle r_N^2 \rangle^{1/2}$ of the isotopes
- number of electrons in the atom or ion

4.2 Examples

The Test Run output contains calculations of the specific mass shift parameter and the electron density for the $1s^22s^21S$ and $1s^22s2p^1P$ states in $B\ II$. The configuration expansions have been obtained by single, double, triple and quadruple excitations to the $3s2p1d$ active set of orbitals. The initial wavefunctions have been obtained from earlier runs. From the parameters obtained for these two states the transition energies are calculated for the isotopes with masses 10 and 11 u.
TEST RUN OUTPUT

========> Case 1 1s(2)2s(2) 1S.

>> lsgen

========> Obtain configuration list

New list, add to existing list, expand existing list, optimized sorting,
restored order or quit? (*/a/e/s/r/q)

> Breit or MCHF? (B/*)

> Default, symmetry or user specified ordering? (*/s/u)

> Highest principal quantum number, n? (1..15)

> Highest orbital angular momentum, l? (s..d)

> Are all these nl-subshells active? (n/*)

> Limitations on population of n-subshells? (y/*)

> Highest n-number in reference configuration? (1..3)

> Number of electrons in 1s? (0..2)

> Number of electrons in 2s? (0..2)

> Number of electrons in 2p? (0..6)

> Resulting term? (1S, 3P, etc.)

> 1S

> Number of excitations = ? (0..4)

> 63 configuration states have been generated.

> Generate a second list? (y/*)

> 63 configuration states in the final list.

The generated file is called clist.out.

>> mv clist.out clist

========> Move clist.out clist

>> ynonh

NEW(ALL=0), N-ZERO(ALL=0)

>0,0

========> Obtain energy expression

>> yspmchfiso

ATOM, TERM, Z in FORMAT(A,A,F) :

>BI,1S,5.

Enter the number of the eigenvalue

>1

========> Obtain radial functions and integrals
There are 6 orbitals as follows:

1s 2s 2p 3s 3p 3d

Enter orbitals to be varied: (ALL,NONE,SOME,NIT=,comma delimited list)

>all

Default electron parameters? (Y/N)

>y

Default values for other parameters? (Y/N)

>y

>> mv cfg.out 3s2p1d1S.c

===== Move cfg.out to 3s2p1d1S.c

>> mv wfn.out 3s2p1d1S.w

===== Move wfn.out to 3s2p1d1S.w

>> mv gradint 3s2p1d1S.g

===== Move gradint (contains the radial integrals needed to calculate the specific mass shift) to 3s2p1d1S.g

>> yisonew

====== Calculation of the specific mass shift parameter

Name of state

>3s2p1d1S

Input from an MCHF (M) or CI (C) calculation?

>m

>> cat 3s2p1d1S.i

===== Display the 3s2p1d1S.i file

================================
Specific mass shift parameter S
================================

Contributions to the parameter from G and R integrals (in a.u.)

-7.9945671579629302E-02 G integrals
0.705128694066368 R integrals

Total value of S (in a.u.)

0.6251830278270075

Total value of S (in cm⁻¹)

68605.90706986833

>> hfsdens

====== Calculation of the electron density

Name of state

>3s2p1d1S
Hyperfine structure and electron density calculation

Electron density at the nucleus? (Y/N)
> y
Hyperfine structure calculation? (Y/N)
> n
Input from an MCHF (M) or CI (C) calculation?
> m
Contributions from different configuration subspaces (Y/N)
> n

>> cat 3s2p1d1S.h
===== Display the 3s2p1d1S.h file

==============================
Electron density calculation
==============================

Electron density at the nucleus (a.u.-3)

J   J
0   0   72.49048445

===== Case 2 1s(2)2s(1)2p(1) 1P.

>> lsgen
===== Obtain configuration list
New list, add to existing list, expand existing list, optimized sorting, restored order or quit? (*/a/e/s/r/q)
> Breit or MCHF? (B/*)
> Default, symmetry or user specified ordering? (*/s/u)
> Highest principal quantum number, n? (1..15)
> 3
Highest orbital angular momentum, l? (s..d)
> d
Are all these nl-subshells active? (n/*)
> Limitations on population of n-subshells? (y/*)
> Highest n-number in reference configuration? (1..3)
> 2
Number of electrons in 1s? (0..2)
> 2
Number of electrons in 2s? (0..2)
> 1
Number of electrons in 2p? (0..6)
> 1
Resulting term? (1S, 3P, etc.)
>1P
Number of excitations = ? (0..4)
>4
98 configuration states have been generated.
Generate a second list? (y/n)
>
98 configuration states in the final list.
The generated file is called clist.out.

>> mv clist.out clist
======> Move clist.out clist

>> ynonh
NEW(ALL=0), N-ZERO(ALL=0)
>0,0

======> Obtain energy expression

>> yspmchfiso
ATOM, TERM, Z in FORMAT(A,A,F) :
>BII,1P,5.
Enter the number of the eigenvalue
>1

There are 6 orbitals as follows:
  1s 2s 2p 3s 3p 3d
Enter orbitals to be varied: (ALL,NONE,SOME,NIT=,comma delimited list)
>all
Default electron parameters? (Y/N)
>y
Default values for other parameters? (Y/N)
>y

>> mv cfg.out 3s2p1d1P.c
======> Move cfg.out to 3s2p1d1P.c

>> mv wfn.out 3s2p1d1P.w
======> Move wfn.out to 3s2p1d1P.w

>> mv gradint 3s2p1d1P.g
======> Move gradint (contains the radial integrals needed to calculate the specific mass shift) to 3s2p1d1P.g

>> yisonew
======> Calculation of the specific mass shift parameter

Name of state
>3s2p1d1P
Input from an MCHF (M) or CI (C) calculation?
>m

>> cat 3s2p1d1P.i
======> Display the 3s2p1d1P.i file
Specific mass shift parameter S

Contributions to the parameter from G and R integrals (in a.u.)

-0.4426032127994707  G integrals
0.7340438759260572   R integrals

Total value of S (in a.u.)
0.2914406631265865

Total value of S (in cm⁻¹)
31981.91595242094

>> hfsdens  =======> Calculation of the electron density
Name of state
>3s2p1d1P

Hyperfine structure and electron density calculation

Electron density at the nucleus ? (Y/N)
>y
Hyperfine structure calculation ? (Y/N)
>n
Input from an MCHF (M) or CI (C) calculation ?
>m
Contributions from different configuration subspaces (Y/N)
>n

>> cat 3s2p1d1P.h  =======> Display the 3s2p1d1P.h file

Electron density calculation

Electron density at the nucleus (a.u⁻³)

<table>
<thead>
<tr>
<th>J</th>
<th>J</th>
</tr>
</thead>
</table>
| 1 | 1  | 70.69252181

===== Case 3 transition isotope shift

>>isosupport
Specify the transition
\[ 1s(2)2s(2) \text{ IS} - 1s(2)2s(1)2p(1) \text{ IP in BII} \]
Nuclear charge
\[ > 5 \]
Energy (a.u.) infinite nucl. mass for lower state
\[ > -24.296413 \]
Energy (a.u.) infinite nucl. mass for upper state (1) or energy diff. (cm\(^{-1}\)) between upper and lower state (2)
\[ > 1 \]
Energy (a.u.) infinite nucl. mass for upper state
\[ > -23.988668 \]
Value of sms parameter S (a.u.) for lower state
\[ > 0.62518 \]
Value of sms parameter S (a.u.) for upper state
\[ > 0.29144 \]
Electron density (a.u.\(^{-3}\)) at the nucleus for lower state
\[ > 72.490 \]
Electron density (a.u.\(^{-3}\)) at the nucleus for upper state
\[ > 70.692 \]
Number of isotopes
\[ > 2 \]
Isotope label (character\#4)
\[ > 10B \]
Isotope mass (u)
\[ > 10.012937 \]
Root mean square nuclear radius sqrt(<r\(^2\)>) (fm)
\[ > 2.44 \]
Isotope label (character\#4)
\[ > 11B \]
Isotope mass (u)
\[ > 11.009305 \]
Root mean square nuclear radius sqrt(<r\(^2\)>) (fm)
\[ > 2.38 \]
Number of electrons
\[ > 4 \]

```plaintext
>>cat isodata

========> Display isodata file containing information about the isotope shift

=================
Initial data
=================

Transition
1s(2)2s(2) IS - 1s(2)2s(1)2p(1) IP in BII

Nuclear charge  5.0000000000000000

Energy (a.u.) infinite nucl. mass for lower state  -24.29641300000000  H
Energy for upper state from calculation
Energy (a.u.) infinite nucl. mass for upper state  -23.98866800000000  H

Value of sms parameter S (a.u.) for lower state  0.6251800000000000  H
```

14
Value of sum parameter $S$ (a.u.) for upper state $0.2914400000000000$ H

Electron density (a.u.$^{-3}$) at the nucleus for lower state $7.490000000000000$ H
Electron density (a.u.$^{-3}$) at the nucleus for upper state $70.69199999999999$ H

Number of isotopes $2$

Isotope label, isotopemass (u) and root mean square nuclear radius (fm)

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Mass (u)</th>
<th>RMS Nuclear Radius (fm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10B</td>
<td>10.012937000000000</td>
<td>2.4400000000000000</td>
</tr>
<tr>
<td>11B</td>
<td>11.009305000000000</td>
<td>2.3800000000000000</td>
</tr>
</tbody>
</table>

Number of electrons $4$

Nuclear mass for the isotopes

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Mass (u)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10B</td>
<td>10.010194100485000</td>
</tr>
<tr>
<td>11B</td>
<td>11.006562100485000</td>
</tr>
</tbody>
</table>

----------

Lower state

----------

Energy for infinite nuclear mass

-24.29641300000000 H

Energy corrected for normal mass effect

10B -24.29508157791551 H
11B -24.29520209876772 H

Energy corrected for normal and specific mass effect

10B -24.29504731672334 H
11B -24.29517093906675 H

Energy corrected for normal and specific mass effect and fieldshift

10B -24.29504570279576 H
11B -24.29516940353675 H

----------

Upper state

----------

Energy for infinite nuclear mass

-23.98866800000000 H

Energy corrected for normal mass effect

10B -23.98735344207112 H
11B -23.98747243637330 H

Energy corrected for normal and specific mass effect

10B -23.98733747053996 H
11B -23.98745791066350 H

Energy corrected for normal and specific mass effect and fieldshift

10B -23.98733589664331 H
11B -23.98745641321990 H

15
Energy differences

Energy difference between upper and lower state

Difference for infinite nuclear mass

\[ 0.3077450000000006 \quad \text{H} \]
\[ 67542.22021861674 \quad \text{cm}^{-1} \]

Transition wavelength (Angstrom)

\[ 1480.555416690861 \quad \text{A} \]

Differences with normal mass correction

10B 0.3077281358443998 \quad \text{H}
11B 0.3077296623944186 \quad \text{H}

10B 67538.51896429451 \quad \text{cm}^{-1}
11B 67538.85400329610 \quad \text{cm}^{-1}

Transition wavelength (Angstrom)

10B 1480.636554273079 \quad \text{A}
11B 1480.629209301059 \quad \text{A}

Wavelength difference between the isotopes

10B 11B 7.3449720196094859E-03 \quad \text{A}

Differences with normal and specific mass correction

10B 0.3077098461833820 \quad \text{H}
11B 0.3077130294032457 \quad \text{H}

10B 67534.50484769739 \quad \text{cm}^{-1}
11B 67535.20326422669 \quad \text{cm}^{-1}

Transition wavelength (Angstrom)

10B 1480.724560363894 \quad \text{A}
11B 1480.709247424001 \quad \text{A}

Wavelength difference between the isotopes

10B 11B 1.5312939893874500E-02 \quad \text{A}

Differences with normal and specific mass and field shift correction

10B 0.3077098061524559 \quad \text{H}
11B 0.3077129903168476 \quad \text{H}

10B 67534.49606192466 \quad \text{cm}^{-1}
11B 67535.19490522854 \quad \text{cm}^{-1}

Transition wavelength (Angstrom)

10B 1480.724752995960 \quad \text{A}
11B 1480.709430695047 A

Wavelength difference between the isotopes
10B 11B 1.532230912885113E-02 A
Part II
Large-scale active space calculations of isotope shifts

5 Introduction
The major problem in MCHF calculations is the selection of the configuration expansion. In accurate calculations it must be possible to estimate the uncertainty of a calculated parameter. Therefore, a whole series of calculations has to be done, where the configuration space is increased in a systematic way.

6 Active space approach
An efficient way of choosing the configuration expansion is to use an active set of radial orbitals. In this approach CSFs of a particular parity and $LS$ symmetry are generated by excitations from one or more reference configurations to the active set. The active set of orbitals is then increased in a systematic way, allowing the convergence of calculated parameters to be studied. By imposing different restrictions on the way excitations can be done, orbitals can be targeted to describe different electron correlation effects. This idea has been utilized by quantum chemists in the restricted active space (RAS) approach for some time [12, 13]. By allowing only single (S) excitations from closed shells in the reference configuration, the orbitals in the active set will describe core-polarization effects. By allowing double (D) excitations, core-correlation in the pair-approximation can be described.

Generally, a good starting point for calculations is to include all single and double excitations to the active set from a few important reference configurations. This can be considered as the zero-order approximation. Since the specific mass shift operator couples configurations that differs with up to two electrons, it is necessary to include triple (T) and quadruple (Q) excitations to improve the wavefunction further. When triple and quadruple excitations are included, the configuration expansion grows very rapidly with the increasing active set of orbitals, and it is in general only possible to include a small subset of these configurations. Another way of including certain triple and quadruple excitations is to use a multi-reference (MR) expansion. Here single and double excitations are made from a set of configurations with expansion coefficients larger than a certain cut-off. The convergence of the calculated parameter can then be studied with respect to the increasing size of the multi-reference set.

7 Active space studies of isotope shifts in boron
7.1 $1s^22s^2\,^1S$ and $1s^22s2p\,^1P$ in $B\,^1I$
If all excitations to the active set are allowed, the configuration expansion, referred to as the complete active space (CAS), grows very rapidly with the increasing active set. Many of these configurations, obtained mainly from triple and quadruple excitations, have very small expansion coefficients and
contribute little to the total energy or to the studied parameters. It is therefore possible to impose restrictions on the allowed excitations, keeping the number of configuration states down, that result in only a very small change in the final result [14, 15].

In the calculations below (from reference [18]) only configurations where at least two of the orbitals have principal quantum numbers \( n < 4 \) were included. In Table I the value of the specific mass shift parameter, the electron density at the nucleus and the total energy, calculated from the zero-order Hamiltonian, for the \( ^1S \) term are shown as a function of the increasing active set of orbitals. It is seen that the specific mass shift parameter is converged to within 0.2 \%. The final value \( S = 0.597 \) a.u. is in very good agreement with the value \( S = 0.597 \) a.u. of Chung et al. [16]. To see the effect of the imposed restrictions on the configuration expansion a CAS calculation was performed for the \( 5s4p3d2f1g \) orbital set. The change in the specific mass shift parameter compared with the restricted expansion is only \( 3 \times 10^{-5} \) a.u. and is of no significance. In Table II the value of the specific mass shift parameter, the electron density at the nucleus and the total energy for the \( ^1P \) term are shown. The specific mass shift parameter changes with 0.5 \% when going from the \( 6s5p4d3f2g1h \) to the \( 7s6p5d4f3g2h1i \) active set, indicating a little slower convergence for the \( ^1P \) term.

In Table III the mass and field shift corrected energies are shown for the \( ^{10}B \) and \( ^{11}B \) isotopes. The field shift corrections were calculated with root mean square nuclear radii; \( ^{10}B, \langle r_N^2 \rangle^{1/2} = 2.44(6) \) fm and \( ^{11}B, \langle r_N^2 \rangle^{1/2} = 2.38(4) \) fm taken from pionic and muonic X-ray measurements [17]. It is seen, as expected for a light atom like boron, that the mass shift is the totally dominating effect. From these energies the wavenumbers and wavelengths for the \( 1s^22s^2 \, ^1S - 1s^22s2p \, ^1P \) transition were determined, the result is shown in Table IV. No experimental value of the isotope shift is known for this transition.

7.2 \( 1s^22s^22p \, ^2P, 1s^22s^23s \, ^2S \) and \( 1s^22s2p \, ^2D \) in \( B \)

Although neutral boron has only five electrons it remains a challenge to calculate the isotope shift accurately. One of the reasons for this is the large and cancelling contributions to the SMS from the \( 1s \) and \( 2s \) shells. This type of cancelling effect is well known for the Fermi contact term where triple excitations change the degree of cancellation between the \( 1s \) and \( 2s \) shell contributions [19]. For SMS the situation is more difficult since the the SMS operator is a two-particle operator whereas the hfs operator is a one-particle operator. This means that in order to describe the degree of cancellation between the \( 1s \) and \( 2s \) shell contributions triple and quadruple excitations have to be included, leading to very large configuration expansions. Another problem is a number of near degeneracies occurring for all three terms studied. To yield quantitatively correct results excitations have to be made from all of these almost degenerate configurations.

Using a MR-MCHF approach where all SD excitations were made from the most important configurations a number of orbital basis sets were obtained. Three- and four-particle effects were then taken into account in large MR-CI calculations where SD excitations to the increasing active sets were done from all CSFs with expansion coefficients larger than 0.01. In Tables V-X the convergence of the SD-MR-MCHF and SD-MR-CI calculations are shown (from reference [20]). The correlation in the \( 1s \) shell is very important for the SMS. This can be seen from the CI calculations where only excitations from the outer shells to the active set were allowed. A comparison with the corresponding calculations were excitations from all shells were allowed shows that the contributions
to the SMS from the CSFs describing the 1s and 2s shell correlation, respectively, are both large but partly cancelling. Thus, a small change in the 1s and 2s shell correlation, due to the inclusion of three and four-particle effects, can have a large influence on the total value of the SMS.

It is seen that the triple and quadruple excitations included in the MR-CI expansion increase the specific mass shift parameter of the $^2P$ term by more than 10%. This change is even larger for the $^2D$ term where the increase is almost 50%. In Table XI the mass and field shift corrected energies are shown for the $^{10}B$ and $^{11}B$ isotopes. The wavenumbers and wavelengths for the $1s^22s^22p$ $^2P$ - $1s^22s^23s$ $^2S$ and $1s^22s^22p$ $^2P$ - $1s^22s2p$ $^2D$ transitions are shown in Table XII. Finally, the transition isotope shifts are compared with values from a third order MBPT calculation and experiment in Table XIII. The calculated isotope shift agrees very well with the experimental shift for both transitions. The present results are encouraging, showing that it is indeed possible to calculate isotope shifts for light atoms with high accuracy.

Since the Hubble Space Telescope was launched there has been an increasing interest in isotope shifts for light atoms due to the possibility of abundance and isotope composition determinations in astrophysical objects. For many transitions experimental data is not available, and the analysis of stellar spectra has to rely on computed isotope shifts [18]. It is reasonable to believe that large-scale MCHF and CI calculations will be of great importance for this work.

Acknowledgement

The authors want to thank Dr Jörgen Carlsson for valuable comments. This research has been supported by the Division of Chemical Science, Office of Basic Energy Sciences, Office of Energy Science, U.S. Department of Energy and by the Swedish Natural Science Research Council.
Table I. The specific mass shift parameter, electron density at the nucleus and total energy (in a.u.) for the $1s^22s^2\, ^1S$ term in $B\, II$ as a function of the increasing active set of orbitals. The total energy has been calculated from the zero-order Hamiltonian. Ncfg is the number of configuration states in the wavefunction expansion.

| active set | $S$ (a.u.) | $|\psi(0)|^2$ | $E_0$ (a.u.) | Ncfg |
|------------|-----------|-------------|-------------|------|
| hf         | 0.000 00  | 72.629     | -24.237 575 | 1    |
| 2s1p       | -0.020 17 | 72.452     | -24.296 413 | 5    |
| 3s2p1d     | 0.625 18  | 72.490     | -24.334 812 | 63   |
| 4s3p2df    | 0.624 81  | 72.497     | -24.342 409 | 460  |
| 5s4p3d2flg | 0.601 69  | 72.501     | -24.346 046 | 1066 |
| 5s4p3d2flg$^a$ | 0.601 66  | 72.501     | -24.346 052 | 2432 |
| 6s5p4d3f2g1h | 0.598 03  | 72.503     | -24.347 410 | 2306 |
| 7s6p5d4f3g2hli | 0.597 09  | 72.504     | -24.347 943 | 2400 |

$^a$ Complete active space calculation. No restriction on the excitations.

Table II. The specific mass shift parameter, electron density at the nucleus and the total energy (in a.u.) for the $1s^22s2p\, ^1P$ term in $B\, II$ as a function of the increasing active set of orbitals. The total energy has been calculated from the zero-order Hamiltonian. Ncfg is the number of configuration states in the wavefunction expansion.

| active set | $S$ (a.u.) | $|\psi(0)|^2$ | $E_0$ (a.u.) | Ncfg |
|------------|-----------|-------------|-------------|------|
| hf         | -0.403 98 | 70.752      | -23.912 873 | 1    |
| 2s1p       | -0.401 07 | 70.748      | -23.913 062 | 4    |
| 3s2p1d     | 0.291 44  | 70.692      | -23.988 668 | 98   |
| 4s3p2df    | 0.256 36  | 70.714      | -24.001 844 | 713  |
| 5s4p3d2flg | 0.277 32  | 70.712      | -24.008 886 | 2300 |
| 5s4p3d2flg$^a$ | 0.277 34  | 70.712      | -24.008 921 | 5654 |
| 6s5p4d3f2g1h | 0.274 59  | 70.717      | -24.011 624 | 5211 |
| 7s6p5d4f3g2hli | 0.273 30  | 70.719      | -24.012 990 | 9772 |

$^a$ Complete active space calculation. No restriction on the excitations.
Table III. The mass and field shift corrected energies for the $1s^22s^21S$ and $1s^22s2p\,^1P$ terms in $B\,II$. The energies are given for the two stable isotopes $^{10}B$ and $^{11}B$.

<table>
<thead>
<tr>
<th>Energy</th>
<th>$1s^22s^21S$</th>
<th></th>
<th>$1s^22s2p,^1P$</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$^{10}B$</td>
<td>$^{11}B$</td>
<td>$^{10}B$</td>
<td>$^{11}B$</td>
</tr>
</tbody>
</table>

Table IV. Calculated spectroscopic data for the resonance transition in $B\,II$. The wavenumbers ($\sigma$) and wavelengths ($\lambda$) are given for the two stable isotopes $^{10}B$ and $^{11}B$.

<table>
<thead>
<tr>
<th>transition</th>
<th>$\sigma$ (cm$^{-1}$)</th>
<th>$\lambda$ (Å)</th>
<th>isotope</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1s^22s^21S - 1s^22s2p,^1P$</td>
<td>73505.735</td>
<td>1360.4381</td>
<td>$^{10}B$</td>
</tr>
<tr>
<td></td>
<td>73506.453</td>
<td>1360.4248</td>
<td>$^{11}B$</td>
</tr>
</tbody>
</table>
Table V. The specific mass shift parameter, electron density at the nucleus and the total energy (in a.u.) for 1s^22s^22p^2P in B I from SD-MR{1s^22s^22p, 1s^22p^3} MCHF calculations.

| n  | \( \mathcal{S} \) (a.u.) | \( |\psi(0)|^2 \) | \( E_0 \) (a.u.) | \( N_{\text{cfg}} \) |
|----|-----------------|-----------------|--------------|-----------|
| hf | -0.404 86       | 71.921          | -24.529 061 | 1         |
| 2  | -0.410 51       | 71.785          | -24.560 354 | 6         |
| 3  | 0.293 90        | 71.792          | -24.621 891 | 129       |
| 4  | 0.240 37        | 71.862          | -24.638 486 | 520       |
| 5  | 0.256 62        | 71.852          | -24.645 478 | 1301      |
| 6  | 0.254 43        | 71.856          | -24.648 728 | 2584      |
| 7  | 0.253 27        | 71.859          | -24.650 290 | 4479      |
| 8  | 0.252 11        | 71.861          | -24.651 009 | 7096      |
| 8^a | -0.361 33      | 72.000          | -24.601 789 | 988       |

^a SD-MR{1s^22s^22p, 1s^22p^3} CI calculation. 1s shell closed and excitations to the active set only allowed from the 2s and 2p shells in the multi-reference configurations.

Table VI. The specific mass shift parameter, electron density at the nucleus and the total energy (in a.u.) for 1s^22s^22p^2P in B I from SD-MR-CI calculations as a function of the increasing active set of orbitals. The multi-reference set consisted of all CSFs with \( c_j > 0.01 \).

| n  | \( \mathcal{S} \) (a.u.) | \( |\psi(0)|^2 \) | \( E_0 \) (a.u.) | \( N_{\text{cfg}} \) |
|----|-----------------|-----------------|--------------|-----------|
| 2  | -0.410 51       | 71.785          | -24.560 354 | 6         |
| 3  | 0.308 97        | 71.791          | -24.622 672 | 366       |
| 4  | 0.258 53        | 71.864          | -24.639 807 | 4520      |
| 5  | 0.275 75        | 71.855          | -24.647 000 | 16525     |
| 6  | 0.274 12        | 71.859          | -24.650 392 | 39623     |
| 6^a | 0.274 12        | 71.859          | -24.650 392 | 17672     |
| 7^b | 0.273 34        | 71.861          | -24.651 991 | 24082     |
| 8^b | 0.272 32        | 71.863          | -24.652 725 | 32456     |

^a The n=6 MR-CI expansion is condensed. Only CSFs with \( c_j > 0.000001 \) are included.
^b CSFs obtained from SD excitations from 1s^22s^22p, 1s^22p^3 and 1s^22s2p3d have been added to the condensed n=6 expansion.
**Table VII.** The specific mass shift parameter, electron density at the nucleus and the total energy (in a.u.) for $1s^22s^23s^2S$ in $B$ from SD-MR\{1s$^2$2s$^2$3s, 1s$^2$2p$^2$3s, 1s$^2$2s2p$^2$\} MCHF calculations.

| n  | $S$ (a.u.) | $|\psi(0)|^2$ | $E_0$ (a.u.) | Ncfg |
|----|-----------|---------------|-------------|------|
| hf | 0.00000   | 72.716        | -24.352 104 | 1    |
| 3  | 0.640 20  | 72.461        | -24.438 718 | 92   |
| 4  | 0.628 00  | 72.535        | -24.456 608 | 379  |
| 5  | 0.625 71  | 72.540        | -24.464 056 | 943  |
| 6  | 0.602 99  | 72.543        | -24.467 945 | 1854 |
| 7  | 0.602 96  | 72.544        | -24.469 218 | 3182 |
| 8  | 0.601 82  | 72.544        | -24.469 860 | 4997 |
| 8$^a$ | -0.024 79 | 73.406         | -24.420 083 | 635  |

$^a$ SD-MR\{1s$^2$2s$^2$3s, 1s$^2$2p$^2$3s, 1s$^2$2s2p$^2$\} CI calculation. 1s shell closed and excitations to the active set only allowed from the 2s, 2p and 3s shells in the multi-reference configurations.

**Table VIII.** The specific mass shift parameter, electron density at the nucleus and the total energy (in a.u.) for $1s^22s^23s^2S$ in $B$ from SD-MR-CI calculations as a function of the increasing active set of orbitals. The multi-reference set consisted of all CSFs with $c_j > 0.01$.

| n  | $S$(a.u.) | $|\psi(0)|^2$ | $E_0$ (a.u.) | Ncfg |
|----|-----------|---------------|-------------|------|
| 3  | 0.640 36  | 72.461        | -24.438 727 | 150  |
| 4  | 0.632 78  | 72.534        | -24.456 917 | 1 734 |  
| 5  | 0.631 31  | 72.539        | -24.464 460 | 5 909 |
| 6  | 0.608 98  | 72.542        | -24.468 409 | 13 431 |
| 7  | 0.609 50  | 72.543        | -24.469 729 | 25 183 |
| 8  | 0.608 55  | 72.543        | -24.470 389 | 41 987 |
Table IX. The specific mass shift parameter, electron density at the nucleus and the total energy (in a.u.) for $1s^22s^2p^2 2D$ in $B\ I$ from SD-MR{$1s^22s2p^2$, $1s^22s^23d$} MCHF calculations.

| n  | S(a.u.) | $|\psi(0)|^2$ | $E_0$ (a.u.) | Ncfg |
|----|---------|--------------|--------------|------|
| hf | -0.736 72 | 70.553       | -24.311 869 | 1    |
| 2  | -0.735 66 | 70.552       | -24.311 921 | 4    |
| 3  | -0.670 12 | 70.740       | -24.379 506 | 157  |
| 4  | -0.065 85 | 70.841       | -24.424 768 | 2320 |
| 5  | -0.066 09 | 70.819       | -24.429 451 | 5004 |
| 6  | -0.069 50 | 70.819       | -24.431 353 | 9161 |
| 7  | -0.658 55 | 70.890       | -24.382 926 | 1530 |

* SD-MR{$1s^22s2p^2$, $1s^22s^23d$} CI calculation. 1s shell closed and excitations to the active set only allowed from the 2s, 2p and 3d shells in the multi-reference configurations.

Table X. The specific mass shift parameter, electron density at the nucleus and the total energy (in a.u.) for $1s^22s^2p^2 2D$ in $B\ I$ from SD-MR-CI calculations as a function of the increasing active set of orbitals. The multi-reference set consisted of all CSFs with $c_j > 0.01$.

| n  | S(a.u.) | $|\psi(0)|^2$ | $E_0$ (a.u.) | Ncfg |
|----|---------|--------------|--------------|------|
| 3  | -0.668 34 | 70.740       | -24.380 038 | 449  |
| 4  | -0.039 40 | 70.878       | -24.418 061 | 7237 |
| 5  | -0.039 01 | 70.846       | -24.426 635 | 32012|
| 6a | -0.038 47 | 70.824       | -24.431 399 | 21674|
| 7a | -0.041 36 | 70.824       | -24.433 330 | 31336|

* The n=5 MR-CI expansion is condensed. Only CSFs with $c_j > 0.000001$ are included. CSFs obtained from SD excitations from $1s^22s2p^2$, $1s^22s^23d$ and $1s^22p^23d$ have been added to the condensed n=5 expansion.
Table XI. The mass and field shift corrected energies for the $1s^22s^22p$ $^2P$, $1s^22s^23s$ $^2S$ and $1s^22s2p^2$ $^2D$ terms in $B\,I$. The energies are given for the two stable isotopes $^{10}B$ and $^{11}B$.

<table>
<thead>
<tr>
<th>Energy</th>
<th>$1s^22s^22p$ $^2P$</th>
<th>$1s^22s^23s$ $^2S$</th>
<th>$1s^22s2p^2$ $^2D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{nm}$</td>
<td>-24.651 374</td>
<td>-24.469 048</td>
<td>-24.431 991</td>
</tr>
<tr>
<td>$E_{nm+sm}$</td>
<td>-24.651 359</td>
<td>-24.469 015</td>
<td>-24.431 993</td>
</tr>
<tr>
<td>$E_{nm+sm+fs}$</td>
<td>-24.651 358</td>
<td>-24.469 013</td>
<td>-24.431 992</td>
</tr>
</tbody>
</table>

Table XII. Calculated spectroscopic data for the resonance transitions in $B\,I$. The wavenumbers ($\sigma$) and wavelengths ($\lambda$) are given for the two stable isotopes $^{10}B$ and $^{11}B$.

<table>
<thead>
<tr>
<th>transition</th>
<th>$\sigma$ (cm$^{-1}$)</th>
<th>$\lambda$ (Å)</th>
<th>isotope</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1s^22s^22p$ $^2P$ - $1s^22s^23s$ $^2S$</td>
<td>40041.8532</td>
<td>2497.3869</td>
<td>$^{10}B$</td>
</tr>
<tr>
<td></td>
<td>40041.6856</td>
<td>2497.3974</td>
<td>$^{11}B$</td>
</tr>
<tr>
<td>$1s^22s^22p$ $^2P$ - $1s^22s2p^2$ $^2D$</td>
<td>47850.5996</td>
<td>2089.8379</td>
<td>$^{10}B$</td>
</tr>
<tr>
<td></td>
<td>47851.1788</td>
<td>2089.8127</td>
<td>$^{11}B$</td>
</tr>
</tbody>
</table>

Table XIII. Transition isotope shift for the resonance transitions. $\Delta \sigma = \sigma_{^{11}B} - \sigma_{^{10}B}$.

<table>
<thead>
<tr>
<th>transition</th>
<th>$\Delta \sigma$ (cm$^{-1}$)</th>
<th>reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1s^22s^22p$ $^2P$ - $1s^22s^23s$ $^2S$</td>
<td>-0.168</td>
<td>MR-CI this work</td>
</tr>
<tr>
<td></td>
<td>-0.094</td>
<td>MBPT</td>
</tr>
<tr>
<td></td>
<td>-0.175</td>
<td>Experiment</td>
</tr>
<tr>
<td>$1s^22s^22p$ $^2P$ - $1s^22s2p^2$ $^2D$</td>
<td>0.579</td>
<td>MR-CI this work</td>
</tr>
<tr>
<td></td>
<td>0.569</td>
<td>Experiment</td>
</tr>
</tbody>
</table>

References


END

DATE

7/6/94

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