

Hartree-Fock and MP2 energy calculation

1.0

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# Chapter 1

## File Index

### 1.1 File List

Here is a list of all files with brief descriptions:

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## Chapter 2

# File Documentation

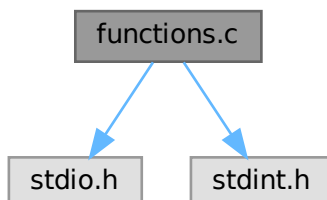
### 2.1 functions.c File Reference

Contains the functions associated with the HF and MP2 energy calculation.

```
#include <stdio.h>
```

```
#include <stdint.h>
```

Include dependency graph for functions.c:



#### Functions

- double [one\\_electron\\_energy](#) (double \*data, int32\_t n\_up, int32\_t mo\_num)
- double [hartree\\_ock\\_energy](#) (double nuc\_repul, double one\_el\_energy, double two\_el\_energy)  
*Calculates the total Hartree-Fock energy.*
- double [get\\_integral](#) (int i, int j, int k, int l, const int32\_t \*index, const double \*value, int64\_t n\_integrals)  
*Retrieves integral value.*

#### 2.1.1 Detailed Description

Contains the functions associated with the HF and MP2 energy calculation.

## 2.1.2 Function Documentation

### 2.1.2.1 `get_integral()`

```
double get_integral (
    int i,
    int j,
    int k,
    int l,
    const int32_t * index,
    const double * value,
    int64_t n_integrals )
```

Retrieves integral value.

#### Parameters

<i>i</i>	First index
<i>j</i>	Second index
<i>k</i>	Third index
<i>l</i>	Fourth index
<i>index</i>	Array containing four-index combinations
<i>value</i>	Array containing integral values
<i>n_integrals</i>	Total number of integrals

#### Returns

Value of the requested integral or 0.0 if not found

### 2.1.2.2 `hartree_fock_energy()`

```
double hartree_fock_energy (
    double nuc_repul,
    double one_el_energy,
    double two_el_energy )
```

Calculates the total Hartree-Fock energy.

#### Parameters

<i>nuc_repul</i>	Nuclear repulsion energy
<i>one_el_energy</i>	One-electron energy contribution
<i>two_el_energy</i>	Two-electron energy contribution

#### Returns

Total Hartree-Fock energy



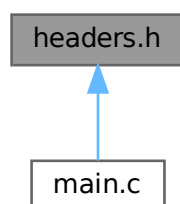
### 2.1.2.3 one\_electron\_energy()

```
double one_electron_energy (
    double * data,
    int32_t n_up,
    int32_t mo_num )
```

## 2.2 headers.h File Reference

Contains the function headers.

This graph shows which files directly or indirectly include this file:



### Functions

- double [one\\_electron\\_energy](#) (double \*data, int32\_t n\_up, int32\_t mo\_num)
- double [two\\_electron\\_energy](#) (int32\_t \*index, double \*value, int32\_t n\_up, int64\_t n\_integrals)  
*Calculates the two-electron energy contribution to the Hartree-Fock energy.*
- double [hartree\\_fock\\_energy](#) (double nuc\_repul, double one\_el\_energy, double two\_el\_energy)  
*Calculates the total Hartree-Fock energy.*
- double [get\\_integral](#) (int i, int j, int k, int l, const int32\_t \*index, const double \*value, int64\_t n\_integrals)  
*Retrieves integral value.*
- double [MP2\\_energy\\_correction](#) (int32\_t \*index, double \*value, double \*mo\_energy, int32\_t n\_up, int64\_t n\_integrals)  
*MP2 energy correction calculation.*

### 2.2.1 Detailed Description

Contains the function headers.

## 2.2.2 Function Documentation

### 2.2.2.1 `get_integral()`

```
double get_integral (
    int i,
    int j,
    int k,
    int l,
    const int32_t * index,
    const double * value,
    int64_t n_integrals )
```

Retrieves integral value.

#### Parameters

<i>i</i>	First index
<i>j</i>	Second index
<i>k</i>	Third index
<i>l</i>	Fourth index
<i>index</i>	Array containing four-index combinations
<i>value</i>	Array containing integral values
<i>n_integrals</i>	Total number of integrals

#### Returns

Value of the requested integral or 0.0 if not found

### 2.2.2.2 `hartree_fock_energy()`

```
double hartree_fock_energy (
    double nuc_repul,
    double one_el_energy,
    double two_el_energy )
```

Calculates the total Hartree-Fock energy.

#### Parameters

<i>nuc_repul</i>	Nuclear repulsion energy
<i>one_el_energy</i>	One-electron energy contribution
<i>two_el_energy</i>	Two-electron energy contribution

#### Returns

Total Hartree-Fock energy

### 2.2.2.3 MP2\_energy\_correction()

```
double MP2_energy_correction (
    int32_t * index,
    double * value,
    double * mo_energy,
    int32_t n_up,
    int64_t n_integrals )
```

MP2 energy correction calculation.

#### Parameters

<i>index</i>	Array containing four-index combinations
<i>value</i>	Array containing integral values
<i>mo_energy</i>	Array of molecular orbital energies
<i>n_up</i>	Number of occupied orbitals
<i>n_integrals</i>	Total number of integrals

#### Returns

MP2 energy correction

Variable used by [MP2\\_energy\\_correction\(\)](#) while calculating the MP2 energy

### 2.2.2.4 one\_electron\_energy()

```
double one_electron_energy (
    double * data,
    int32_t n_up,
    int32_t mo_num )
```

### 2.2.2.5 two\_electron\_energy()

```
double two_electron_energy (
    int32_t * index,
    double * value,
    int32_t n_up,
    int64_t n_integrals )
```

Calculates the two-electron energy contribution to the Hartree-Fock energy.

#### Parameters

<i>index</i>	Array containing four-index combinations for two-electron integrals
<i>value</i>	Array containing values of two-electron integrals
<i>n_up</i>	Number of occupied orbitals
<i>n_integrals</i>	Total number of two-electron integrals

## Returns

Two-electron energy contribution

Variable used by [two\\_electron\\_energy\(\)](#) while calculating the two-electron interaction energy

## 2.3 headers.h

[Go to the documentation of this file.](#)

```

00001
00006 #ifndef FUNCTIONS_H
00007 #define FUNCTIONS_H
00008
00009 double one_electron_energy(double* data, int32_t n_up, int32_t mo_num);
00010 double two_electron_energy(int32_t* index, double* value, int32_t n_up, int64_t n_integrals);
00011 double hartree_fock_energy(double nuc_repul, double one_el_energy, double two_el_energy);
00012
00013 double get_integral(int i, int j, int k, int l, const int32_t* index, const double* value, int64_t
n_integrals);
00014 double MP2_energy_correction(int32_t* index, double* value, double* mo_energy, int32_t n_up, int64_t
n_integrals);
00015
00016 #endif
00017

```

## 2.4 main.c File Reference

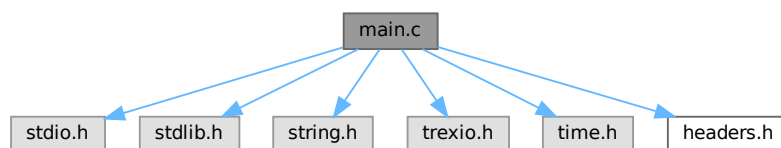
Contains the main program.

```

#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <trexio.h>
#include <time.h>
#include "headers.h"

```

Include dependency graph for main.c:



### 2.4.1 Detailed Description

Contains the main program.

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