# 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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2 File Index

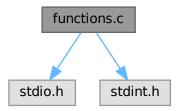
## **Chapter 2**

### **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 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.

#### 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 1,
    const int32_t * index,
    const double * value,
    int64_t n_integrals )
```

Retrieves integral value.

#### **Parameters**

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

#### Returns

Value of the requested integral or 0.0 if not found

#### 2.1.2.2 hartree\_fock\_energy()

Calculates the total Hartree-Fock energy.

#### **Parameters**

nuc_repul	Nuclear repulsion energy
one_el_energy	One-electron energy contribution
two_el_energy	Two-electron energy contribution

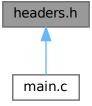
Returns

Total Hartree-Fock energy

#### 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)
  - Calculates the one-electron energy contribution to the Hartree-Fock 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.
- 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()

Retrieves integral value.

#### **Parameters**

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

#### Returns

Value of the requested integral or 0.0 if not found

#### 2.2.2.2 hartree\_fock\_energy()

Calculates the total Hartree-Fock energy.

#### **Parameters**

nuc_repul	Nuclear repulsion energy
one_el_energy	One-electron energy contribution
two_el_energy	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

index	Array containing four-index combinations
value	Array containing integral values
mo_energy	Array of molecular orbital energies
n_up	Number of occupied orbitals
n_integrals	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()

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

#### **Parameters**

data Array containing one-electron integr		Array containing one-electron integrals
	n_up	Number of occupied orbitals
	mo_num	Total number of molecular orbitals

#### Returns

One-electron energy contribution

Variable used by one\_electron\_energy() while calculating the one-electron energy

#### 2.2.2.5 two\_electron\_energy()

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

#### **Parameters**

index	Array containing four-index combinations for two-electron integrals
value	Array containing values of two-electron integrals
n_up Number of occupied orbitals	
n_integrals	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

#### 2.3 headers.h

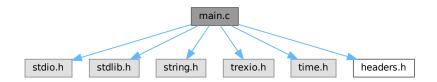
Go to the documentation of this file.

```
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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