

XMHFL

Software for calculating excited and ionized states of molecules

The software is based on the solvation of the system of coupled integro-differential equations for all MO constituting the electron configuration of the state. The higher harmonics of MO are represented in the form of the composition of expanded into the series of wave functions of atomic electron shells in accord with spherical harmonics. It ensures the necessary description accuracy of electron density in the neighborhood of molecular system nuclears. The offered calculation procedure is based on the combination of three-point difference Numerov scheme and Thomas algorithm.

THEORY

XMHFL

Basic equation of iteration scheme

Integro-differential equations make the basis of the iteration scheme of obtaining the radial parts. They are the generalization of Hatree-Fock equations recorded for an atom for the first time [1]. The equations are obtained on the basis of minimizing the energy functional in Born-Oppenheimer [2] approximation for the wave function on N-electron molecular system $\Psi = (N!)^{-1/2} \det \|\phi_{n\gamma}\|$, represented as antisymmetrized product of one-electron MO $\phi_{n\gamma}$. After the variation procedure we obtain a set of coupled integro-differential Hartree-Fock equations systems every of which corresponds the definite MO $n\gamma$ of molecule electron configuration. The one-electron MO $\phi_{n\gamma}$, in nonrelativistic SC representation has the form [3]:

$$\Phi_{n\gamma\mu}(r, \vartheta, \varphi) = \frac{1}{r} \sum_l P_l^{n\gamma}(r) Y_l^\mu(\vartheta, \varphi), \quad (1)$$

где $P_l^{n\gamma}(r)$ – radial and $Y_l^\mu(\vartheta, \varphi)$ – angle part of partial harmonic l – symmetry of MO with the fixed (for a linear molecule) value μ – projections of impulse moment on the axis of quantization OZ (molecule axis), n – main quantum number, γ – symmetry of MO and r, ϑ, φ – spherical coordinates.

Considering (1) the system of coupled integro-differential equations for MO $n\gamma$ has the form:

$$\frac{d^2 P_l^{n\gamma}(r)}{dr^2} = \sum_{l'} \Omega_{l,l'}^{n\gamma}(r) P_{l'}^{n\gamma}(r) + 2X_l^{n\gamma}(r), \quad (2)$$

where $\Omega_{l,l'}^{n\gamma}(r)$ – local potential, describing the electron interaction of MO $n\gamma$ with the nuclears of molecular system and direct Coulomb interaction with electrons of other MO, $X_l^{n\gamma}(r)$ nonlocal potential, describing exchange Coulomb interaction of electrons of MO $n\gamma$ with electrons of other MO.

Local potential $\Omega_{l,l'}^{n\gamma}(r)$ has the following form:

$$\Omega_{l,l'}^{n\gamma}(r) = \left[\frac{l(l+1)}{r^2} - \frac{2Z_0}{r} - \varepsilon_{n\gamma} \right] \delta_{l,l'} + 2W_{l,l'}^{n\gamma}(r) + 2V_{l,l'}^{n\gamma}(r), \quad (3)$$

where Z_0 – the charge of molecular nuclear, located in the chosen origin of coordinates, $W_{l,l'}^{n\gamma}(r)$ – the potential of crystal field, describing the electron interaction of MO $n\gamma$ with the nuclears of molecular system, $V_{l,l'}^{n\gamma}(r)$ – the potential of direct Coulomb interaction of electrons of MO $n\gamma$ with the electrons of other MO, $\varepsilon_{n\gamma}$ – one electron energy $n\gamma$ of MO.

The expression for the potential of crystal field (3) has the form:

$$W_{l,l'}^{n\gamma}(r) = \sum_{\mu} \lambda_{\mu}^{n\gamma} \omega_{l,l'}^{n\gamma\mu}(r), \quad (4)$$

$$\omega_{l,l'}^{n\gamma\mu}(r) = - \sum_{\alpha=1}^{N_L} Z_{\alpha} \sum_{k=|l-l'|}^{l+l', \Delta k=2} C_{l_{\mu} l'_{\mu}}^k C_0^{k*}(\theta_{\alpha}, \varphi_{\alpha}) \left(\frac{r_{\alpha <}^k}{r_{\alpha >}^{k+1}} \right), \quad (5)$$

where $\lambda_{\mu}^{n\gamma}$ – a number of electrons of MO $n\gamma$ with μ – projection of the impulse moment on the quantization axis OZ (molecule axis); N_L – a number of ligands in the molecule, Z_{α} – the charge of α –th ligand; $C_m^l = \sqrt{4\pi/2l+1} Y_{lm}(\theta, \varphi)$ – spherical harmonic; $r_{\alpha >} = \max(r, R_{\alpha})$ and $r_{\alpha <} = \min(r, R_{\alpha})$, $R_{\alpha}, \theta_{\alpha}, \varphi_{\alpha}$ – the coordinates of the α –th ligand; $C_{l_{\mu} l'_{\mu}}^k$ – matrix element of the spherical harmonic, the methods of calculation of which are described in [2].

The potential, describing the direct Coulomb interaction of electrons $n\gamma$ with the electrons from other MO (3) has the form:

$$V_{l,l'}^{n\gamma}(r) = \sum_{n'\gamma'} (1 + \delta_{n\gamma, n'\gamma'}) \alpha_{n'\gamma'}^{n\gamma} \cdot F_{l,l'}^{n'\gamma'}(r), \quad (6)$$

$$F_{l,l'}^{n'\gamma'}(r) = \frac{1}{r} \sum_{l_1, l_2}^{k_{max}, \Delta k=2} C_{l_1 l_2}^k C_{l' l}^k Y_{l_1 l_2 k}^{n'\gamma'}(r), \quad (7)$$

where $\alpha_{n'\gamma'}^{n\gamma}$ – the coefficient for the potential describing the direct Coulomb interaction between $n\gamma$ and $n'\gamma'$ MO depending on the quantum number of electron configuration of a molecule, $k_{min} = \max(|l-l'|, |l_1-l_2|)$, $k_{max} = \min(l+l', l_1+l_2)$.

Nonlocal potential describing the interchange Coulomb interaction of electrons, $n\gamma$ of MO with the electrons of other MO in (2) has the form:

$$X_l^{n\gamma}(r) = \sum_{n'\gamma'} \beta_{n'\gamma'}^{n\gamma} \sum_{l'} G_{l,l'}^{n\gamma, n'\gamma'}(r), \quad (8)$$

$$G_{l,l'}^{n\gamma, n'\gamma'}(r) = \frac{1}{r} \sum_{l_1, l_2}^{k_{max}, \Delta k=2} C_{l_1 l'}^k C_{l_2 l}^k Y_{l_1 l' k}^{n'\gamma', n\gamma}(r) P_{l_2}^{n'\gamma'}(r), \quad (9)$$

where $\beta_{n'\gamma'}^{n\gamma}$ – the coefficient for the potential describing interchange Coulomb interaction between $n\gamma$ and $n'\gamma'$ of MO depending on the quantum number of electron configuration of a molecule, $k_{min} = \max(|l_1-l'|, |l_2-l|)$, $k_{max} = \min(l_1+l', l+l_2)$.

The radial part of electron potential is determined in the expressions for direct and interchange potentials. It is calculated on the basis of radial parts of partial harmonics of SC expansion of MO:

$$Y_{l_1 l_2 k}^{S,R}(r) = \left(\int_0^r \left[\frac{x}{r} \right]^k + \int_r^\infty \left[\frac{r}{x} \right]^{k+1} \right) P_{l_1}^S(x) P_{l_2}^R(x) dx, \quad (10)$$

In order to simplify the expressions (6)-(9) the omission of summing on the μ -projection of impulse moment of electrons participating in Coulomb interaction is done.

The inclusion of higher spherical harmonics in SC expansion of MO

For accurate description of electron density in the neighborhood of molecular system nuclei and solvation of the problem of slow convergence of functional series (1) of MO $n\gamma$ when calculating the system of connected differential equations the following form is given:

$$\Phi_{n\gamma\mu}(r, \vartheta, \varphi) = A_{n\gamma\mu} \left[\frac{1}{r} \sum_{l=l_{min}}^{l_0} P_l^{n\gamma}(r) Y_l^{\mu}(\vartheta, \varphi) + \sum_{n'\gamma L} \Lambda_{\mu}^{n'\gamma L} \psi_{\mu l_0}^{n'\gamma L}(r) \right], \quad (11)$$

where $A_{n\gamma\mu}$ – normalizing factor, $\Lambda_{\mu\alpha}^{n\gamma L}$ – contribution factor of the wave function $\psi_{\mu l_0}^{n\gamma L}(r)$ – with the main quantum number n and assymetry γ L – th ligand of molecular system has the form:

$$\psi_{\mu l_0}^{n\gamma L}(r) = \frac{1}{r} \sum_{l > l_0} P_l^{n\gamma L}(r) Y_l^\mu(\vartheta, \varphi), \quad (12)$$

The functions $\psi_{\mu l_0}^{n\gamma L}(r)$ are expanded into a series in spherical harmonics of wave functions of electron shells of the atoms that are included into the molecular system as ligands (atoms that are not located in the origin of coordinates).

In this case, partial harmonics of MO in (11) with the values of orbital moment $l \leq l_0$ are obtained via the solvation of the system of equations (2). Expansion terms (11) with orbital moments $l > l_0$ are obtained on the basis of linear combination $\psi_{\mu l_0}^{n\gamma L}(r)$ with the contribution factor $\Lambda_{\mu\alpha}^{n\gamma L}$. Such a representation of MO is explained by the fact that the form of partial spherical harmonics with big values of orbital moment is determined to the accuracy of the ratio by the potential of a molecular system ligand.

The choice of value l_0 in (11) is made in the result of numerical experiment and depends on the character of molecular system and on the number of partial harmonics participating in the formation of chemical bond of the composition.

In order to determine the contribution factors $\Lambda_{\mu\alpha}^{n\gamma L}$ in (11) sewing of partial harmonics is done, the equation:

$$P_{l_0}^{n\gamma}(r) = \sum_{n'\gamma L} \Lambda_{\mu\alpha}^{n'\gamma L} P_{l_0}^{n'\gamma L}(r), \quad (13)$$

That is, radial part of l_0 –th partial harmonic of $n\gamma$ – molecular orbital is represented in the form of superposition of radial partial harmonics of ligand functions with weight factors $\Lambda_{\mu\alpha}^{n\gamma L}$.

The expression (13) enables to make up a system of algebraic equations for determining the contribution factors $\Lambda_{\mu\alpha}^{n\gamma L}$ of ligand functions with symmetry γ in the form of:

$$\sum_{n'\gamma L} \langle P_{l_0}^{j\gamma L} | P_{l_0}^{n'\gamma L} \rangle \Lambda_{\mu\alpha}^{n'\gamma L} = \langle P_{l_0}^{j\gamma L} | P_{l_0}^{n\gamma} \rangle, \quad (14)$$

The determined, thus, MO is normed per unit.

EFSH

The expansion of the wave functions of the electron shells of an atom in a series of spherical harmonics

The procedure of obtaining ligand functions $\psi_{\mu l_0}^{n\gamma L}(r)$ is based on recalculation of wave functions of electron shells of atoms $P_{nl}^A(r)$, included into the molecular system in a new unified system of coordinates.

Within the process of transition into a unified system of coordinates the wave function of an electron shell related to the definite atom is represented in the form of expansion into a series in spherical harmonics [4]:

$$\Phi_{nlm}^A(r, \vartheta, \varphi) = \sum_{L=0}^{\infty} \Gamma_{LM}^{nlm}(R) Y_{LM}(\Xi, \phi), \quad (15)$$

where $\Phi_{nlm}^A(r, \vartheta, \varphi)$ – wave function nl – of electron shell in the atomic system of coordinates; r, ϑ, φ – spherical coordinates of the atomic system; $\Gamma_{LM}^{nlm}(R)$ – expansion ration in spherical harmonics in the molecular spherical system of coordinates; L –orbital moment of expansion of a wave function in the molecular system of coordinates; M –projection of an orbital moment in the molecular system of coordinates; R, Ξ, ϕ – spherical coordinates in a molecular system.

Expansion ratio series (15) can be represented in the form [4]:

$$\Gamma_{LM}^{nlm}(R) = \int_0^\pi \frac{P_n^A(r)}{r} \Theta_{LM}(\vartheta) \Theta_{LM}(\Xi) \sin \Xi d\Xi, \quad (16)$$

$$\Theta_{lm}(\beta) = \sin(\beta)^m \sum_{s=0}^{l-m} T_s^{lm} \cos(s\beta), \quad (17)$$

$$r^2 = R^2 + R_M^2 - 2RR_M \cos\varphi_{12}, \quad (18)$$

$$\cos \vartheta = (R \cos \Xi - R_M \cos Y)/r, \quad (19)$$

$$\cos\varphi_{12} = \cos(\Xi) \cos(Y) + \sin(\Xi) \sin(Y) \cos(\phi - F), \quad (20)$$

where R_M, Y, F – the coordinates of the location of the point of coordinates origin of molecular system in the atomic system, T_s^{lm} – coefficients of representing of theta-function in trigonometrical form.

On the basis of the expressions (17) and of the formulas (18)-(19) connecting the coordinates in different systems the integration is done in (16). That enables to expand the wave functions of electron shells of atoms relating the chosen molecular center.

GenAF module. Generation of wave functions of an atomic ligand.

1. It is necessary to create a file (ATTITLE.DAT) with a list of service files and their location on the hard disk
2. It is necessary to generate a file (GeneratorAF.DAT) with input data

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! NcoeffCalculLagran-parameter indicating the addition of off-diagonal factors
! NcoeffCalculLagran = 0 - there are no off-diagonal factors
! NcoeffCalculLagran = 1 - calculation taking into account off-diagonal factors
! NtipSetky-MESH TYPE
! NtipSetky = 1-ATOMIC GRID
! NtipSetky = 2-MOLECULAR GRID
READ(3,*)Z,IS,NtipSetky,BET,GAMMA,RAL,N,H,R,EPS,IZAP,IOUT,IFUNC,IPOT,NFK,NGK,NDP,NZ,NONREL,IPKOEf,NcoeffCalculLagran
! enter electronic configuration
READ(3,*)(NN(I),L(I),Q(I),NST(I),I=1,IS)
! EXTERNAL POTENTIAL COEFFICIENTS
NUF=1
ACY=0
VAL=0
IF(RAL.GT.1.D-3) THEN
    READ(3,*) NUF,ACY,VAL
    READ(3,*)(ISD(I),KD(I),DEL(I),I=1,NUF)
END IF

! ENTERING THE COEFFICIENTS OF THE COULON INTERACTION
IF(NGK.NE.0) THEN
    DO I=1,NGK
        READ(3,*) IX(1,I),IY(1,I),K(1,I),DCOFF(1,I)
    ENDDO
ENDIF

IF(NFK.NE.0) THEN
    DO I=1,NFK
        READ(3,*) IX(2,I),IY(2,I),K(2,I),DCOFF(2,I)
    ENDDO
ENDIF
```

EFSH module is the transformation of the wave functions of atomic ligands in the transition from atomic to the unified molecular coordinate system

1. It is necessary to create a file (TITLE.DAT) with a list of service files and their location on the hard disk
2. It is necessary to generate a file (EFSH.DAT) with input data

! Numerical data input block

! Ral-distance from the atomic coordinate system to the decomposition center coordinate system

! Ral> 0 - displacement occurs along the OZ axis (IN POSITIVE DIRECTION)

! Ral <0 - offset occurs against the OZ axis (IN NEGATIVE DIRECTION)

! Lmax-orbital moment of the last term in which the expansion is performed

! NtipSetkyatom-mesh type for expandable function

! NtipSetky-type mesh

! NtipSetky = 1-ATOMIC GRID

! NtipSetky = 2-MOLECULAR GRID (GRID FOR THE CASE OF NON-COINCIDENCE OF THE BEGINNING OF THE SYSTEM OF COORDINATES WITH THE ATOM)

! NKie-CONDITION FOR RECORDING DECOMPOSITION COEFFICIENTS

! NKie = 0-DECOMPOSITION RATES ARE NOT WRITTEN TO FILE

! NKie = 1-DECOMPOSITION COEFFICIENTS WRITE TO FILE

! IZFUN-NUMBER OF THE FIRST RECORD INTO FILE DECOMPOSITION COEFFICIENT

READ(5,*) Z, IS, NtipSetkyatom, NtipSetky, NKie

XMHFL.

1. It is necessary to create a file (MTTITLE.DAT) with a list of service files and their location on the hard disk.

!! DATA FILE NAME

READ (5, '(A90)') DATFIL

!! FILE FILE NAME IN WHICH CALCULATION RESULT WILL BE WRITTEN

READ (5, '(A90)') FILE1

!! FILE NAME OF CALCULATION RESULTS

READ (5, '(A90)') OUTFIL

!! FILE NAME OF INTERMEDIATE RESULTS OF HARMONIZATION (SINGLE-ELECTRONIC ENERGIES OF MOLECULAR ORBITALS)

READ (5, '(A90)') OUTFILEOE

!! FILE NAME IN WHICH COEFFICIENTS OF MIXING LIGANDA FUNCTIONS AT EVERY ITERATION WILL BE RECORDED

READ (5, '(A90)') OUTFILAlfaLigands

!! FILE NAME IN WHICH THE SEARCH OF THE SOLUTION OF THE SYSTEM OF EQUATIONS IS WRITTEN

READ (5, '(A90)') OUTFILSEARCHE

!! FILE NAME IN WHICH DEPENDENCE OF THE INTEGRAL OF ORTHOGONALITY FROM ENERGY IS RECORDED

!! IN THE EVENT OF ROOT ABSENCE

READ (5, '(A90)') OUTFILSPECTRUME

!! FILE NAME FILE CONTAINING ZERO APPROXIMATION

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READ (5, '(A90)') FILEZERO
!! FILE NAME FOR RECORDING INTERIM RESULTS
READ (5, '(A90)') FUNBuffer
READ (5, '(A90)') FUNBuffer1
READ (5, '(A90)') FUNBuffer2
READ (5, '(A90)') FUNBuffer3
READ (5, '(A90)') FUNBuffer4
!! FILE NAME IN WHICH FUNCTIONS OF LIGANDS RECORDED
READ (5, '(A90)') FILELigands
!! FILE NAME IN WHICH DATA ABOUT ELECTRONIC DENSITY IS RECORDED
READ (5, '(A90)') FileElectronicDensity
!! FILE NAME IN WHICH NORMAL PERMANENT RECORDED
READ (5, '(A90)') FileMORnorm
!! FILE NAME IN WHICH POTENTIALS WILL BE WRITTEN
READ (5, '(A90)') FilePOT
!! FILE NAME IN WHICH PARAMETERS CORRECT THE WORK OF THE PROGRAM
READ (5, '(A90)') FileParameterCorrection

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2. It is necessary to generate a file (XMHFL.DAT) with input data.

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!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!! BLOCK OF DATA INPUT !!!!!!!!!!!!!!!!!!!!!!!
!! INTRODUCING INFORMATION ABOUT CONFIGURATION OF MOLECULE NUCLEI
!! Nnuclei-NUMBER OF NUCLEI (DO NOT CONSIDER NUCLEAR AT THE BEGINNING OF THE COORDINATE)
77 READ(3,*) Nnuclei

!! INTRODUCE THE CONFIGURATION OF MOLECULE NUCLEI
!! Z0-CHARGE OF THE NUCLEI AT THE BEGINNING OF THE COORDINATE
!! Z (Nnuclei) -MASSIVE CHARGES OF NUCLEI
!! CoorR (Nnuclei) -MASSIVE RADIAL COORDINATES
!! CoorR (Nnuclei) -RADIAL NUCLEAR COORDINATE (R-RADIUS)
!! CoorA (Nnuclei, 2) -MASSIVE NORDIC COORDINATE
!! CoorA (Nnuclei, 1) -THE COORDINATE -RTeta-ANGLE (0 = <RTeta <= PI)
!! CoorA (Nnuclei, 2) - COORDINATE CO-ORDINATE -RFu-ANGLE (0 = <RFu <= 2 * PI)
!! NFunctionLigand (Nnuclei) -Number of Ligand functions (functions used to describe the higher harmonics of the representation
of a molecular orbital) READ(3,*) Z0
DO IIZ=1,Nnuclei
  READ(3,*) Z(IIZ),CoorR(IIZ),CoorA(IIZ,1),CoorA(IIZ,2),NFunctionLigand(IIZ)
ENDDO

!! CONSIDER THE TYPES OF LIGAND FUNCTIONS
!! Mligands (IIZ, IXID) -MASSIVE OF THE PROJECTS OF LIGANDA FUNCTIONS
!! Nligands (IIZ, IXID) -MASSIVE OF THE MAIN QUANTUM NUMERALS OF LIGAND FUNCTIONS
!! Lligands (IIZ, IXID) -MASSIVE OF ORBITAL QUANTUM NUMBERS
DO IIZ=1,Nnuclei
  READ(3,*) (Mligands(IIZ,IXID),Nnligands(IIZ,IXID),Lligands(IIZ,IXID),IXID=1,NFunctionLigand(IIZ))
ENDDO

!! INTRODUCING CONFIGURATION INFORMATION
!! IndexHartreeFock-PARAMETER INDICATING WHAT EQUATION IS DECIDED
!! IndexHartreeFock = 0-HARTRI EQUATION

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!! IndexHartreeFock = 1-HARTRI-FOCA EQUATION
!! NumbreMO-NUMBER OF MOLECULAR ORBITALS IN CONFIGURATION
!! PARAMETER PARAMETERS
!! ALFA
!! BET
!! GAMMA
!! N is the number of points
!! H-step
!! Rmax-The maximum value of the integration radius
!! EPS-accuracy of calculation (DEVIATION BETWEEN TWO SOLUTIONS)
!! EPSXR-accuracy of calculation (DETERMINATION OF SINGLE-ELECTRON ENERGIES IN DECISION OF EQUATIONS)
!! IZAP-record number for the first harmonic of the first molecular orbital
!! IKLZERO-KEY APPROACHING THE TYPE OF THE NULL APPROACH
!! AT IKLZERO = 0-NUL APPROXIMATION IS "BAD" CALCULATION FOR THE FIRST ITERATION IS IMPLEMENTED
WITHOUT EXCHANGE
!! AT IKLZERO = 1-NUL APPROACH IS A "GOOD" CALCULATION ON THE FIRST ITERATION IS IMPLEMENTED WITH
THE EXCHANGE
!! IreshimSO-PARAMETER INDICATING THE TYPE OF HARMONIZATION OF MOLECULAR ORBITALS
!! IreshimSO = 0-STANDARD MODE OF CODE
!! IreshimSO = 1- "STRENGTHENING" HARMONIZATION MODE THE BINDING COEFFICIENTS ARE EXPRESSED
!! IndexExit-PARAMETER INDICATING EMERGENCY STOPPING OF THE PROGRAM
!! IndexExit = 0-PROGRAM WORKS WITHOUT FAILURES
!! IndexExit = 1-HAS FAILED TO REALIZE INFORMATION FROM EMERGENCY FILES
READ(3,*) IndexHartreeFock,NumbreMO,BET,GAMMA,N,H,Rmax,EPS,EPSXR,IZAP,IKLZERO,IreshimSO,IndexExit
!! INTRODUCE THE ELECTRONIC CONFIGURATION OF MOLECULES
!! NN (NumbreMO) -MASSIVE OF MAIN QUANTUM NUMBERS
!! ML (NumbreMO) -MASSIVE OF MOLECULAR ORBITAL PROJECTIONS
!! IQ (NumbreMO) -MASSIVE NUMBERS OF FILLING (NUMBER OF ELECTRONS ON MOLECULAR ORBITAL)
READ(3,*)(NN(I),ML(I),IQ(I),I=1,NumbreMO)

WRITE(6,1050) (NN(I),LB(IABS(ML(I))+1),IQ(I),I=1,NumbreMO)
WRITE(6,*)

!! We introduce the parameters of the single-center decomposition of molecular orbits
!! NumbreGarmMO (NumbreMO) - MASSIVE NUMBER OF HARMONICS IN THE MOLECULAR ORBITAL
!! NumbreGarmLMO (NumbreMO) - MASSIVE NUMBER OF HARMONICS IN THE MOLECULAR ORBITAL TO LgarmonicMO
(3, NumbreMO) INCLUDING THIS HARMONIC
!! LgarmonicMO (3, NumbreMO) -MASSIVE VALUES OF ORBITAL MOMENTS OF MOLECULAR ORBITALS
!! LgarmonicMO (1, NumbreMO) - MINIMUM VALUE
!! LgarmonicMO (2, NumbreMO) -MAXIMUM VALUE
!! LgarmonicMO (3, NumbreMO) - ORBITAL MOMENT IMPORTANCE AFTER WHICH CALCULATION IS DONE ON
LEGAND FUNCTIONS (functions do not change when solving)
DO I=1,NumbreMO
  READ(3,*) NumbreGarmMO(I),LgarmonicMO(1,I),LgarmonicMO(2,I),LgarmonicMO(3,I)
ENDDO

!! INTRODUCE THE STRUCTURE OF A MOLECULAR ORBITAL CONSTRUCTED FROM THE FUNCTIONS OF LIGANDS
!! NumbreLigand (I) - NUMBER OF LIGANDS OF FUNCTIONS USED FOR A MOLECULAR ORBITAL
!! NLigands (I, II) -MASSIVE OF LIGAND NUMBERS USED FOR MOLECULAR ORBITALS
!! NFunLigands (I, IIXZ) -MASSIVE NUMBER OF FUNCTIONS OF THIS LIGAND USED FOR THIS MOLECULAR ORBITAL
DO I=1,NumbreMO
  READ(3,*) NumbreLigand(I),(NLigands(I,II),II=1,NumbreLigand(I))
  !! WE WRITE THE NUMBERS OF FUNCTIONS
  DO IIXZ=1,NumbreLigand(I)
    READ(3,*) NFunLigands(I,IIXZ),(NumbreFunctionLig(I,IIXZ,IYYZ),IYYZ=1,NFunLigands(I,IIXZ))
  ENDDO
ENDDO

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!! INTRODUCE THE PROJECTIONS OF MOLECULAR ORBITALS AND COEFFICIENTS OF INTERACTION
!! CYCLE ON MOLECULAR ORBITALS
DO I=1,NumbreMO
  !! CYCLE FOR TYPES OF COEFFICIENTS
  DO J=1,NtypIndexCoffNucleusElectron(I)
    READ(3,*) MLNucleusElectron(1,J,I),MLNucleusElectron(2,J,I),RcoeffNucleusElectron(J,I)
  ENDDO
ENDDO

!! ENTER THE NUMBER OF TYPES OF DIRECT CULON INTEGRALS
DO I=1,NumbreMO
  READ(3,*) (NtypIndexCoffF(I,J),J=1,NumbreMO)
ENDDO
!! Let us introduce the number of types of exchangeable Coulomb integrals
DO I=1,NumbreMO
  READ(3,*) (NtypIndexCoffG(I,J),J=1,NumbreMO)
ENDDO

!! INTRODUCTION OF DIRECT CULON INTERACTION COEFFICIENTS
!! MassivMLaf (NtypIndexCoffF, NumbreMO, NumbreMO, 4) -MASSIVE OF Moment (MOLECULAR ORBITAL) PROJECTIONS
WHEN CALCULATING DIRECT INTERACTION
!! RcoeffAF (NtypIndexCoffF, NumbreMO, NumbreMO) -MASIVE OF DIRECT INTERACTION FACTORS
DO I=1,NumbreMO
  DO J=1,NumbreMO
    IF(NtypIndexCoffF(I,J).NE.0) THEN
      DO II=1,NtypIndexCoffF(I,J)
        READ(3,*) MassivMLaf(II,I,J,1),MassivMLaf(II,I,J,2),MassivMLaf(II,I,J,3),MassivMLaf(II,I,J,4),RcoeffAF(II,I,J)
      ENDDO
    ENDIF
  ENDDO
ENDDO

!! INTRODUCTION OF EXCHANGE INTERACTION COEFFICIENTS
!! MassivMLbg (NtypIndexCoffG, NumbreMO, NumbreMO, 4) -MASSIVE OF Moment (MOLECULAR ORBITAL) PROJECTIONS
WHEN CALCULATING EXCHANGE INTERACTION
!! RcoeffBG (NtypIndexCoffG, NumbreMO, NumbreMO) -MASIVE OF EXCHANGE INTERACTION COEFFICIENTS
DO I=1,NumbreMO
  DO J=1,NumbreMO
    IF(NtypIndexCoffG(I,J).NE.0) THEN
      DO II=1,NtypIndexCoffG(I,J)
        READ(3,*) MassivMLbg(II,I,J,1),MassivMLbg(II,I,J,2),MassivMLbg(II,I,J,3),MassivMLbg(II,I,J,4),RcoeffBG(II,I,J)
      ENDDO
    ENDIF
  ENDDO
ENDDO

!! WE WRITE THE MODULE OF THE LOWER ENERGY BORDER
!! MODULE OF THE ENERGY OF THE POINT OF THE POTENTIAL PIT (CONDITIONAL POINT OF REPORT) IN RIDBERGS
(WITHOUT MINUS)
READ(3,*) EzeroXF

!! We introduce the parameters of the single-center decomposition of the Molecular Orbital of a non-zero approximation
!! NumbreGarmMOZero (NumbreMO) - HARMONIC NUMBER OF MASSES IN THE MOLECULAR ORBITAL OF THE NULL
APPROXIMATION
!! LgarmonicMOZero (3, NumbreMO) -MASSIVE OF THE ORBITAL MOMENT VALUES OF MOLECULAR ORBITALS OF THE
ZERO APPROXIMATION
!! LgarmonicMOZero (1, NumbreMO) - MINIMUM VALUE
!! LgarmonicMOZero (2, NumbreMO) -MAXIMUM VALUE
!! LgarmonicMOZero (2, NumbreMO) -MAXIMUM VALUE

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!! LgarmonicMOZero (3, NumbreMO) - ORBITAL MOMENT IMPORTANCE AFTER WHICH CALCULATION IS DONE ON
LEGAND FUNCTIONS (functions do not change when solving)
DO I=1,NumbreMO
    READ(3,*) NumbreGarmMOZero(I),LgarmonicMOZero(1,I),LgarmonicMOZero(2,I),LgarmonicMOZero(3,I)
ENDDO
!! INTRODUCTION ZONES OF RECORDING PARTIAL HARMONICS OF THE NULL APPROACH
!! IZONGarmonZero (NumbreMO, NumbreGarmLMOZero (NumbreMO)) - MASSIVE of ZONES OF RECORDING PARTIAL
HARMONICS OF THE ZERO ACCELERATION TO LgarmonicMOZero (3, NumbreMO) INCLUSIVE
!! IZONGarmonZero (NumbreMO, NumbreGarmLMOZero (NumbreMO)) = 0-MEANS THAT THE PARTIAL HARMONIC IS
EQUAL TO ZERO
    DO I=1,NumbreMO
        READ(3,*) (IZONGarmonZero(I,J),J=1,NumbreGarmLMOZero(I))
    ENDDO
ENDIF
ENDIF

```

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