H–FUNCTION CALCULATION FOR SELECTED SPECTRAL BANDS OF OXYGEN

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1 INTRODUCTION

The Oxygen, from the reason of its uniqueness and irreplaceability in the meaning for the whole life and now in climate-change, is under intensive scientific research, mainly for its absorption properties. The present work deals with the calculation of absorption properties of oxygen molecule with the help of a program using of modern density theory, the basis of which was laid by Enrico Fermi.

2 BASIC RELATIONS

For the purpose of calculating the H-function of the absorption coefficient for oxygen it is necessary to know the force of the oscillator f. Program Orca allows this important physical quantity to be calculated according to the following relation:

$$f = f_D + f_M, \tag{1}$$

where f_D represents the power of the oscillator given by the dipole moment and oscillator force given by the magnetic dipole moment f_M. The absorption coefficient is given by:

$$\kappa(\nu) = N_L B_{LU} h \nu_{LU} F(\nu), \tag{2}$$

where N_L is the occupancy of the lower level, B_{LU} is the Einstein absorption coefficient, ν_{LU} it the frequency of the line, $F(\nu)$ is the line profile.

The H-fuction itself is given by the relation:

$$H_{LU} = \frac{8\pi^3}{3hc} \frac{\omega_I}{\omega_\Lambda (2S+1) Q_{nucl}} \left| R_e^{v''v'} \right|^2 S_{J''} \omega_{LU} \tag{3}$$

where ω_I is the nuclear spin of atoms, ω_Λ statistical weight of the orbital angular moment Λ with respect to the internuclear axis, S is the total electron spin, Q_{nucl} is the kernel part of the partition function, $\left| R_e^{v''v'} \right|$ is vibronic transition moment, $S_{J''}$ are Hoehnl-London factors and ω_{LU} is the wavenumber of the transition.

Program Orca has a wide range of computational functions related to the closed and unclosed shells which are represented by unpaired electrons. An example of calculating the frequency of individual states is shown in fig. 1.

The actual calculation of the H-fuction is performed by the program NKrov2 which I developed, its output shows the H-function, see fig. 2.

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      *** CONVERGENCE OF RESIDUAL NORM REACHED ***
        --- The CIS iterations have converged ---

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UHF CIS RESULTS
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IROOT=  1:  0.176542 au     4.804 eV   38746.5 cm**-1
    5b ->   7b    0.321106 (-0.566662)
    5b ->   8b    0.106447 ( 0.326263)
    5b ->  14b    0.049941 ( 0.223476)
    5b ->  15b    0.014255 ( 0.119396)
    6b ->   7b    0.106447 (-0.326263)
    6b ->   8b    0.321106 (-0.566662)
    6b ->  14b    0.014255 ( 0.119396)
    6b ->  15b    0.049941 (-0.223476)
```

Figure 1: An example of frequency calculation for individual states.

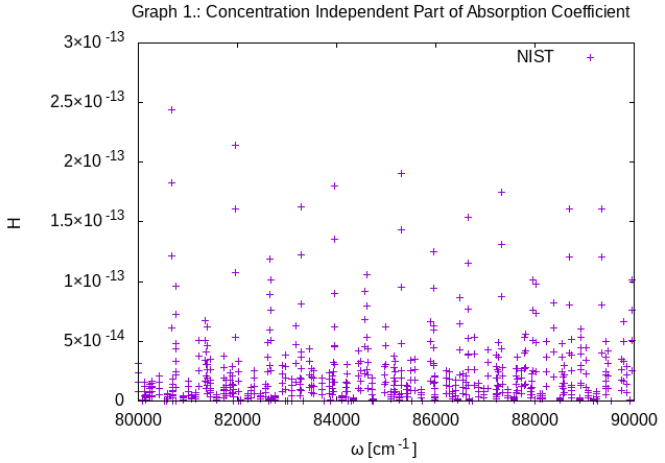

Figure 2: Concentration independent part of (H-function) of the absorption coefficient.

3 CONCLUSION

The use of these programs allows you to tabulate H-fuction which greatly simplifies calculation of the absorption coefficient for subsequent physical research.

ACKNOWLEDGEMENT

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