

Research Article

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Solar Far Infrared-Induced Growth of Plants is Due to Non-Thermal Effect of Infrared to Radio-Frequency Electromagnetic Energy: Verification by Quantum Chemistry Molecular Modeling (DFT/MM)

Shozo Yanagida^{1,2*} and Takeko Matsumura²¹Osaka University, Ibaraki, Japan²Minerva Light Laboratory, Kyoto, Japan**ABSTRACT**

This article shows new properties of positive integers related to the sum of the deviations of the products of dividing the positive number by each of its factors, as well as the positive integer with only three divisors called the perfect square with a square root as a prime number, and the article also shows the building scheme a computer application to find the number of divisors of a number, and to classify the number into prime and composite.

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Introduction

Sunlight includes energy of far-infrared (FIR) ranging from THz, GHz and radio wave. It is considered that far infrared energy (FIR) of sunlight is essential for the growth of plants as learnt of recent literature [1,2]. In other words, FIR must be closely related to the activation of mitochondria, the engine of plant cells. The role of mitochondria is to generate superoxide anion radicals ($O_2^{\cdot-}$), an energetic substance, from oxygen. The contribution of solar FIR to plant growth is the activation of oxygen, i.e., the magnetic loss of triplet oxygen (3O_2) results in conversion to singlet oxygen (1O_2), and results in effective $O_2^{\cdot-}$ formation.

Methodology

Molecular modeling based on density functional theory (DFT/MM) yields theory IR and FIR ($500\sim 0\text{ cm}^{-1}$) spectra of equilibrium geometries of molecular van der Waal aggregates as theory ones. Equilibrium structures of triplet oxygen (3O_2) aggregates containing water (H_2O) and their theory IR/FIR spectra are obtainable by DFT/MM. The magnetic loss of $3O_2$ and the formation of highly active singlet oxygen (1O_2) can be verified by analyzing the intensity change of their theory IR/FIR spectrum.

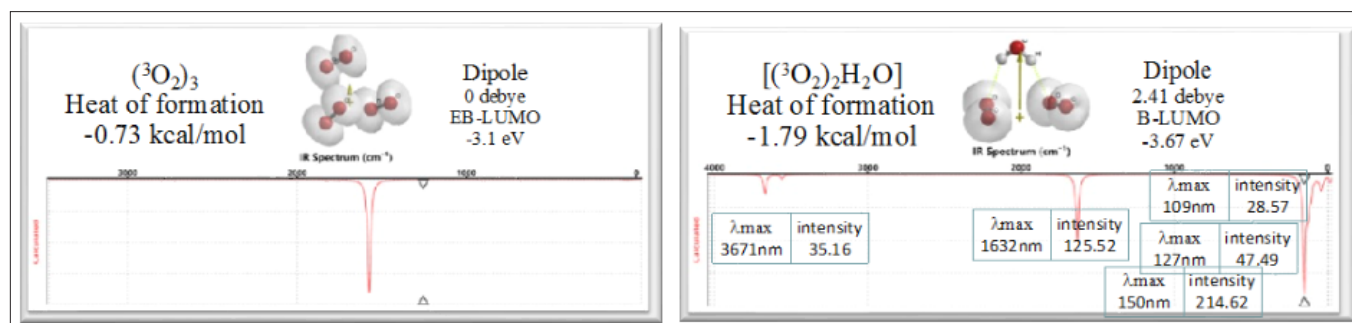


Figure 1: (a): Theory IR/FIR spectra obtained for equilibrium geometry of triplet oxygen trimer ($3O_2$)³. (b): Theory IR/FIR spectrum obtained for equilibrium geometry of hydrated triplet oxygen dimer [$(^3O_2(H_2O)_2)_2$].

Results & Discussion

DFT/MM has been performed on molecules, and it has been verified that many small molecules form trimeric van der Waals aggregates [3].

DFT/MM verifies the theory IR/FIR spectrum of the equilibrium geometry (EQG) of the $^3\text{O}_2$ trimeric van der Waals aggregates ($^3\text{O}_2$)₃ (Figure 1a). The heat of formation of the aggregate, the dipole, and the potential of the lowest unoccupied molecular orbital (EB-LUMO) are obtainable from B-LUMO is an index of oxidation power. EQG is shown together with the spin density on $^3\text{O}_2$. Judging from theory IR/FIR spectrum of ($^3\text{O}_2$)₃, verifies that it does not absorb FIR rays at all. And the small heat of formation indicates that the probability of the formation of ($^3\text{O}_2$)₃ is very low.

Figure 1b shows the DFT/MM-based theory IR/FIR spectrum of EQG obtained for $^3\text{O}_2$ dimer and H_2O van der Waals aggregate [$^3\text{O}_2(\text{H}_2\text{O})_2$], its heat of formation, its dipole and its B-LUMO potential energy (EB-LUMO). The EQG is shown together with the spin density on $^3\text{O}_2$. Judging from the heat of formation, the

probability of its formation is not high. However, remarkable intensity of the absorption maximum (max) for FIR is manifested. In addition, absorption intensity and max of absorption and dissipation of IR can be confirmed. And then, thermo-upconversion mechanism-based thermal effect is confirmed for [$^3\text{O}_2(\text{H}_2\text{O})_2$]. However, the absorption intensity in the IR region does not balance with absorption intensity in the FIR region.

Figure 2a shows the theory IR/FIR spectrum for EQG of the dihydrate 3O_2 van der Waals aggregate of [$^3\text{O}_2(\text{H}_2\text{O})_2$] and its heat of formation, its dipole, and its EB-LUMO. The EQG is shown together with the spin density on $^3\text{O}_2$. Compared with the heat of formation of [$^3\text{O}_2(\text{H}_2\text{O})_2$], its formation probability is the higher. Surprisingly, it has now been shown to absorb strongly far-infrared rays. And the absorption and divergence of infrared rays are remarkable. However, the absorption intensity in the IR region does not reflect the absorption intensity in the IR region. We now come to consider that this will predict and verify not only up-conversion of FIR energy but also the magnetic loss of $^3\text{O}_2$ to $^1\text{O}_2$.

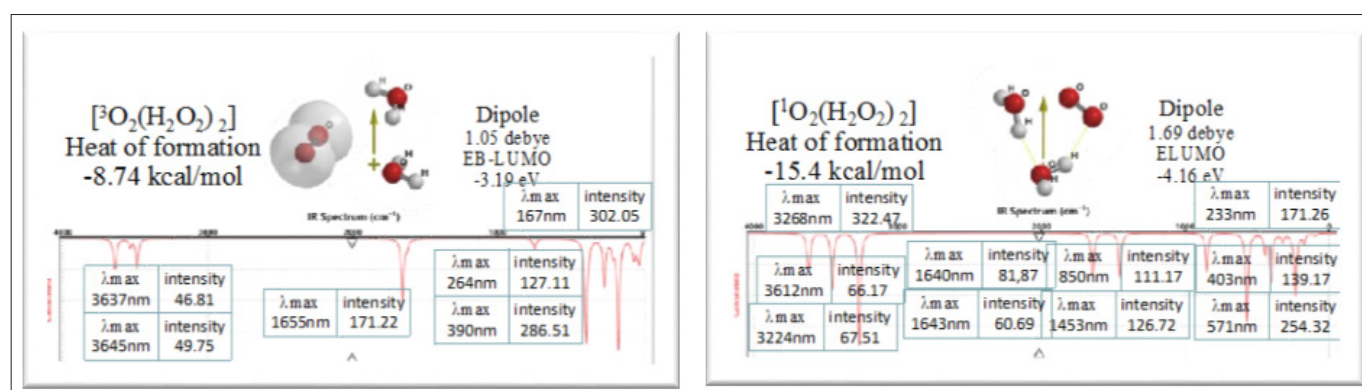


Figure 2: (a): Theory IR/FIR spectrum obtained for equilibrium geometry of di-hydrated triplet oxygen [$^3\text{O}_2(\text{H}_2\text{O})_2$]. (b): Theory IR/FIR spectrum obtained for equilibrium geometry of di-hydrated single oxygen [$^1\text{O}_2(\text{H}_2\text{O})_2$].

This prediction of FIR magnetic loss for [$^3\text{O}_2(\text{H}_2\text{O})_2$] is verified by comparing its IR/FIR spectrum with the IR/FIR spectrum of a water and singlet oxygen ($^1\text{O}_2$) aggregate, [$^1\text{O}_2(\text{H}_2\text{O})_2$].

Figure 2b shows the theory IR/FIR spectrum for EQG of the dihydrate $^1\text{O}_2$ van der Waals aggregate of [$^1\text{O}_2(\text{H}_2\text{O})_2$] with its heat of formation, its dipole, and its ELUMO. The heat of formation indicates the higher probability of formation than that of [$^3\text{O}_2(\text{H}_2\text{O})_2$]. Interestingly, the ELUMO, -4.16 eV is much lower than the BLUMO of [$^3\text{O}_2(\text{H}_2\text{O})_2$], -3.16 eV. This verifies significant increase in oxidizing power of oxygen under FIR irradiation. We now understand that FIR irradiation of mitochondria converts the triplet oxygen aggregates [$^3\text{O}_2(\text{H}_2\text{O})_2$] to the singlet oxygen aggregate [$^1\text{O}_2(\text{H}_2\text{O})_2$]. Furthermore, thermo-upconversion of [$^1\text{O}_2(\text{H}_2\text{O})_2$] and the resulting thermal effect promotes the production of $\text{O}_2^{\cdot -}$ in mitochondria, i.e., activation of mitochondria, i.e., plant cell engine.

Conclusions

Contribution of solar FIR ray to plant growth is due to the activation of triplet oxygen of [$^3\text{O}_2(\text{H}_2\text{O})_2$] to singlet oxygen of [$^1\text{O}_2(\text{H}_2\text{O})_2$]. Magnetic loss should be recognized as a non-thermal effect under THz~GHz~MHz irradiation.

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