Infrared spectrum of planetary-nebula analyzed by pure-carbon graphene molecule

*Norio Ota[1]

1. University of Tsukuba,Graduate school of pure and applied sciences

Planetary nebula is an important candidate to produce many dusts in the space. Especially, carbon-stars as like Tc1 and Lin49 show featured infrared spectrum IR [1]. It was understood that carbon fullerene (C60 and C70) could reproduce similar spectrum [2]. However, there are many extra-bands, still not identified by fullerene. We can see many graphene molecules during synthesis of fullerene in laboratory, which bring an idea to study a possibility of graphene by the first principles calculation.

We tried the quantum chemical calculation starting from model molecule of (C24) having seven carbon-hexagons using the Gaussian09 program. We applied two astrophysical conditions. One is a void creation by high speed proton, another photo-ionization by the central star. Best calculated result was obtained by graphene (C23) molecule having one carbon pentagon combined with six hexagons. Ionized states were sum of neutral, mono- and di-cations.

By an astronomical observation, we can see 16 infrared bands in a wavelength range of 5~25 micrometer [1]. Experimentally confirmed bands of fullerene (sum of C60 and C70) were 8 bands, half numbers of observed bands. In case of graphene (C23), calculated result shows that all of observed 16 bands can be reproduced very well by this calculation [3]. The reason may be high productivity of graphene from carbon gas as reported from laboratory experiments. We can suggest that graphene plays an important role in the atmosphere of the carbon-star.

References

[1] Otsuka M. , et al., Monthly notices of the royal astronomical society, vol.462 issue 1, p-12 (2016)

[2] Cami J. , et al., Science, vol.329, p-1180 (2010)

[3] Norio Ota, arXiv 1811.05043 (2018)

Keywords: planetary nebula, graphene, infrared spectrum

