

Graphene-Molecule Compared with Fullerene-C60 in Carbon-rich Planetary Nebula by Quantum-Chemical Analysis

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It had been understood that astronomically observed infrared spectrum (IR) of carbon-rich planetary nebula comes from fullerene-C60. Whereas, it is well known by on-earth experiments that graphene-molecule is a source material for synthesizing fullerene. It will be simply supposed that graphene-molecule may float in astronomical space. In order to check such assumption, this study compared graphene-molecule with fullerene by the quantum-chemical calculation. Calculated IR's were also compared with observed one of carbon rich planetary nebula Tc 1 and Lin 49. Model graphene molecules are (C23), (C22), and (C21) having few carbon pentagons as shown in Fig.1. Calculated result was amazing that graphene-molecule could reproduce many observed bands as shown in Fig.2, where coincided bands are marked by green dot lines. On the other hand in case of fullerene-C60, calculation could reproduce only major bands, but was too poor to reproduce many detailed bands. We can predict that graphene-molecule may be major carbon material rather than fullerene. We should confirm it by on-earth study using actual graphene-molecules.

Fig.1
Model molecules

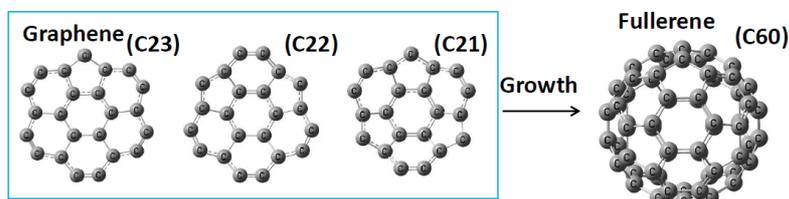


Fig.2,
Observed infrared spectrum identified by calculated bands of graphene and fullerene

