Reproducing interstellar infrared spectrum by modeling a hydrocarbon pentagon-hexagon combined molecule

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Interstellar infrared spectrum coming from polycyclic hydrocarbon molecules shows a ubiquitous pattern in a wavelength of 3-15 micrometer (1). These years, thousand kind of molecules were test and discussed as a candidate. However, any convincing single molecule was not discovered by both experiment and calculation. Here, promising single molecule was studied by quantum-chemistry first principles calculation focusing on hydrocarbon pentagon-hexagon combined molecule parametarizing charge and spin state. Among many candidates, better one was dication (C23H12)+2 having two pentagons and five hexagons (2). Calculated main peaks were 3.2 , 6.4, 7.6, 7.8, 8.6, 11.2, 12.7 and 14.1 micrometer. Those show very good coincidence with astronomically observed values as 3.3, 6.2, 7.6, 7.8, 8.6, 11.2, 12.7, and 14.3 micrometer. Also, another small molecule (C12H8)3+ having one pentagon and two hexagons shows good coincidence at major wavelength of 3.2, 6.4, 7.5, 7.8, and 11.2 micrometer. This is the first case to give good coincidence by a single molecule. References: (1)Christiaan Boersma et al, Astrophysical Journal 690.1208(2009) (2)Norio Ota, arXiv:1402.0009(2014) (3)Norio Ota, arXiv:1510.07403(2015)

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