

# Infrared spectra of protonated and hydrogenated corannulene, $C_{20}H_{11}^+$ and $C_{20}H_{11}$ , in solid *para*-hydrogen and their relationship to interstellar unidentified infrared bands

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Polycyclic aromatic hydrocarbons (PAH) and their derivatives, including protonated and cationic species, are suspected to be carriers of the unidentified infrared (UIR) emission bands observed from the galactic and extra-galactic sources. We extended our investigations of infrared (IR) spectra of protonated planar PAH to a non-planar PAH, corannulene ( $C_{20}H_{10}$ ), which is regarded as a fragment of a fullerene,  $C_{60}$ . The protonated corannulene  $C_{20}H_{11}^+$  was produced on bombarding a mixture of corannulene and *para*-hydrogen (*p*- $H_2$ ) with electrons during deposition at 3.2 K. During maintenance of the electron-bombarded matrix in darkness the intensities of IR lines of protonated corannulene decreased because of neutralization by electrons that was slowly released from the trapped sites. The observed lines were classified into two groups according to their responses to secondary irradiation at 365 nm. Eighteen lines in one group are assigned to the lowest-energy species among five possible isomers, *hub*- $C_{20}H_{11}^+$ , and seventeen in another group to *rim*- $C_{20}H_{11}^+$ , the species of second lowest energy. Spectral assignments were derived based on a comparison of the observed spectra with those predicted with the B3PW91/6-311++G(2d,2p) method [1]. The observed IR spectrum of *hub*- $C_{20}H_{11}^+$  resembles several bands of the Class-A UIR bands.

We also report the IR spectra of hydrogenated corannulene ( $C_{20}H_{11}$ ) in solid *p*- $H_2$ . The hydrogenated corannulene were also generated from electron bombardment of a mixture of corannulene and *p*- $H_2$  during deposition of a matrix at 3.2 K. The features that increased with time after maintaining the matrix in darkness for a long period are assigned to the most stable isomers of hydrogenated corannulene, *hub*- $C_{20}H_{11}$  and *rim*- $C_{20}H_{11}$ , according to behavior of secondary photolysis and comparison with the vibrational wavenumbers and IR intensities predicted with the B3PW91/6-311++G(2d,2p) method. In an alternate method in which we produced hydrogenated corannulene by UV irradiation of a matrix  $C_{20}H_{10}/Cl_2/p$ - $H_2$ , followed by IR irradiation to promote the reaction  $Cl + H_2$  to form H atoms to react with corannulene. In this case we observed all three isomers, *hub*-, *rim*-, and *spoke*- $C_{20}H_{11}$ . This indicates that most *hub*- $C_{20}H_{11}$  and *rim*- $C_{20}H_{11}$  produced during electron bombardment might be from neutralization of protonated corannulene, because only *hub*- and *rim*- $C_{20}H_{11}^+$  were produced in these experiments.

## References

- [1] P. Sundararajan, M. Tsuge, M. Baba & Y.-P. Lee, 2018, ACS Earth Space Chem.  
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