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Supplementary Material

Electronic Spectroscopy of a $C_7H_4^+$ Isomer in a Neon Matrix: Methyltriacetylene Cation

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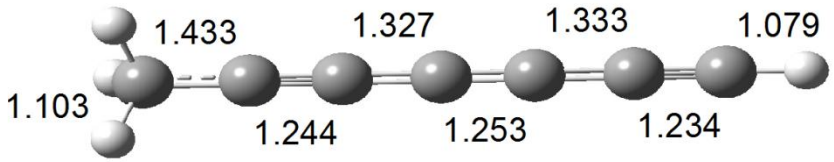

Methyltriacetylene cation (C_{3V})

Table S1. Electronic excitation energies E_{cal} (eV) and oscillator strength (f) of the dipole allowed electronic transitions for methyltriacetylene cation calculated by the CASPT2 method and comparison to the experiment E_{exp} (eV).

Ground state	E_{cal}	f	E_{exp}	Symmetry of States
X ^{2}E (C_{3V})	**2.21**	0.0648	2.06	**1** ^{2}E
	3.34	0.0250	2.96	**2** ^{2}E
	3.58	0.0003		**3** ^{2}E
	4.30	0.0241		**5** ^{2}E
	5.07	0.0003		**6** ^{2}E
	5.91	0.0012		**7** ^{2}E

Table S2. Wavenumbers of the vibrations of methyltriacetylene cation calculated with DFT method using the B3LYP functional and the cc-pVDZ basis set.

a_1 (cm^{-1}): 3410, 3003, 2283, 2242, 2091, 1405, 1348, 977, 539.

e (cm^{-1}): 3108, 1408, 1012, 744, 642, 554, 374, 263, 153.