Table S1. Standard enthalpies of formation at different methods as well as data from NIST [1].

Species		CH_3 (methyl)	C_2H_2 (acetylene)	C_6H_5 (phenyl)	C_8H_6 (phenylacetylene)	$C_{10}H_8$ (naphthalene)	$C_{14}H_{10}$ (anthracene)
M06-2X/6-311+G(d,p)		157.33	247.69	367.03	367.64	208.80	315.14
B2PLYP-D3/def2-TZVPP		148.41	238.79	344.27	331.51	161.52	243.80
CCSD(T)	cc-pVDZ	231.92	378.59	742.86	861.31	820.86	1155.58
	cc-pVTZ	171.17	281.77	495.93[2]	522.88	402.53	581.74
	cc-pVQZ	157.31	255.60	418.87	420.12	272.33[2]	---
	CBS(DZ,TZ)	143.05	236.96	381.63[2]	366.22	208.88	316.11
	CBS(TZ,QZ)	147.69	237.45	365.41	348.82	181.99[2]	---
NIST		147.0±1.0	227.4±0.8	339.0±8.0	306.6±1.7	150.0±10.0	202.2±2.3

Note: All geometries were optimized at M062X/6-311+G(d,p) level, with zero-point energies (ZPEs) calculated at the same level using a scaling factor of 0.97 [3]. Single-point energies were refined using B2PLYPD3 and CCSD(T) methods at M062X optimized geometries. All values are given in kJ/mol.

The references cited in Table S1 are as follows:

[1] Linstrom PJ, Mallard, WG. NIST Chemistry WebBook. In: NIST Standard Reference
Database Number 69. National Institute of Standards and Technology (2018).

[2] Zhang Z, Ye L, Jin H, et al. Kinetic study of the growth of PAHs from biphenyl with the assistance of phenylacetylene[J]. Combustion and Flame, 2025, 272: 113881.

[3] Alecu IM, Zheng J, Zhao Y, et al. Computational thermochemistry: scale factor databases and scale factors for vibrational frequencies obtained from electronic model chemistries[J]. Journal of chemical theory and computation, 2010, 6(9): 2872-2887.