

Supplementary Materials

for

Thermal Stability and Vibrational Properties of the 6,6,12-Graphyne-Based Isolated Molecules and Two-Dimensional Crystal

Ekaterina S. Dolina ¹, Pavel A. Kulyamin ¹, Anastasiya A. Grekova ¹, Alexey I. Kochaev ^{2,3,4}, Mikhail M. Maslov ^{1,2} and Konstantin P. Katin ^{1,2,*}

¹ Institute of Nanotechnologies in Electronics, Spintronics and Photonics, National Research Nuclear University “MEPhI”, Kashirskoe Sh. 31, Moscow 115409, Russia

² Laboratory of Computational Design of Nanostructures, Nanodevices, and Nanotechnologies, Research Institute for the Development of Scientific and Educational Potential of Youth, Aviatorov Str. 14/55, Moscow 119620, Russia

³ Laboratory of Acoustic Microscopy, Science Institute of Biochemical Physics Named after N.M. Emanuel of the Russian Academy of Sciences, Kosygina Str. 4, Moscow 119334, Russia

⁴ Research and Education Center “Silicon and Carbon Nanotechnologies”, Ulyanovsk State University, Leo Tolstoy Str. 42, Ulyanovsk 432017, Russia

* Correspondence: kpkatin@yandex.ru

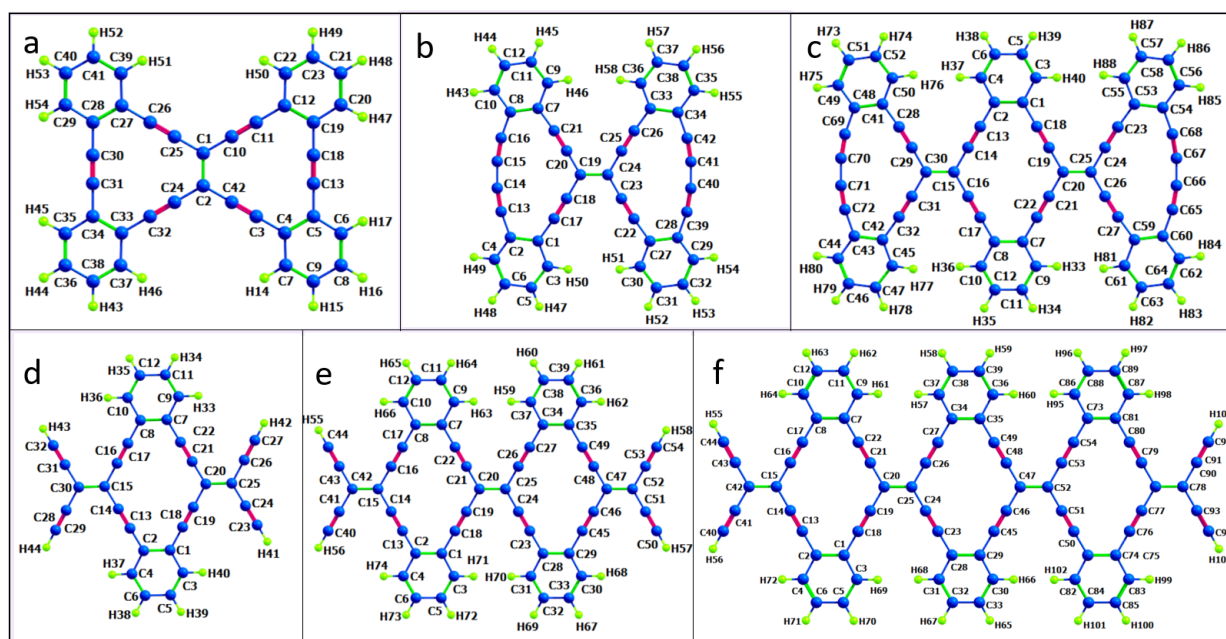


Figure S1. Valence angles of 6,6,12-graphyne-based oligomers: (a) $\underline{O1}$: C(25)-C(1)-C(10) 120.035° ; C(26)-C(25)-C(1) 179.678° ; C(27)-C(26)-C(25) 179.908° ; C(40)-C(41)-C(39) 120.063° ; (b) $\underline{O2}$: C(20)-C(19)-C(18) 119.962° ; C(19)-C(20)-C(21) 178.005° ; C(20)-C(21)-C(7) 176.107° ; C(12)-C(11)-C(9) 120.205° ; C(8)-C(16)-C(15) 169.777° ; C(16)-C(15)-C(14) 170.590° ;

C(15)-C(14)-C(13) **170.568°**; C(14)-C(13)-C(2) **169.699°**; (c) O3: C(29)-C(30)-C(31) **119.918°**; C(30)-C(29)-C(28) **178.000°**; C(41)-C(28)-C(29) **176.197°**; C(16)-C(15)-C(14) **120.153°**; C(15)-C(14)-C(13) **179.769°**; C(14)-C(13)-C(2) **179.941°**; C(6)-C(5)-C(3) **120.043°**; C(48)-C(69)-C(70) **169.744°**; C(69)-C(70)-C(71) **170.508°**; C(70)-C(71)-C(72) **170.513°**; C(71)-C(72)-C(43) **169.762°**; (d) O4: C(26)-C(25)-C(24) **120.058°** [116.02°]; C(21)-C(20)-C(19) **120.183°** [117.45°]; C(20)-C(21)-C(22) **179.808°** [174.6°]; C(21)-C(22)-C(7) **179.892°** [177.8°]; C(20)-C(19)-C(18) **179.927°** [178.6°]; C(19)-C(18)-C(1) **179.769°** [176.56°]; C(12)-C(11)-C(9) **120.069°**; (e) O5: C(53)-C(52)-C(51) **120.050°** [115.74°]; C(25)-C(26)-C(27) **179.569°** [179.30°]; C(26)-C(27)-C(34) **179.878°** [175.8°]; C(25)-C(24)-C(23) **179.530°** [176.52°]; C(24)-C(23)-C(28) **179.917°** [177.9°]; C(26)-C(25)-C(24) **119.969°** [117.91°]; C(47)-C(48)-C(49) **179.683°** [171.3°]; C(48)-C(49)-C(35) **179.782°** [177.5°]; C(47)-C(46)-C(45) **179.723°** [178.8°]; C(46)-C(45)-C(29) **179.743°** [174.2°]; C(48)-C(47)-C(46) **119.737°** [117.59°] C(12)-C(11)-C(9) **120.054°**; (f) O6: C(91)-C(90)-C(93) **120.032°**; C(90)-C(91)-C(92) **179.879°**; C(77)-C(78)-C(79) **119.738°**; C(78)-C(79)-C(80) **179.720°**; C(79)-C(80)-C(81) **179.778°**; C(88)-C(89)-C(87) **119.980°**. The values in square brackets correspond to the experimentally obtained data (see Ref. 22).

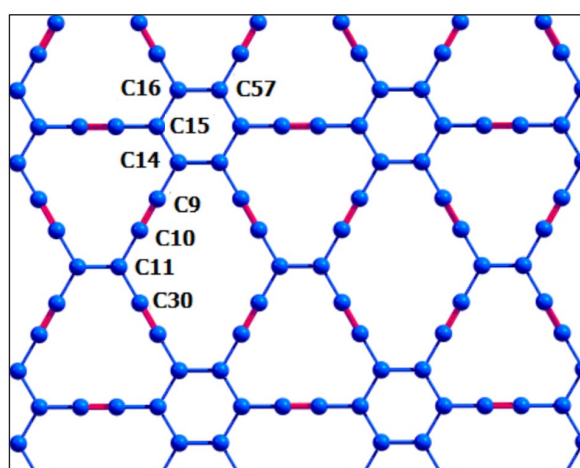


Figure S2. Valence angles of 6,6,12-graphyne crystal: C(30)-C(11)-C(10) **120.384°**; C(11)-C(10)-C(9) **179.952°**; C(10)-C(9)-C(14) **179.578°**; C(15)-C(16)-C(57) **120.315°**.