Synthesis of the Biphenylene Nanoribbon by Compressing the Biphenylene under Extreme Conditions

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Table S1. Assignments of IR modes of biphenylene by density functional theory (DFT) calculation.

Assignments	Calculation (0 K, 0 GPa)	Experiment (0.66 GPa)
Skeletal formation	603	610
Skeletal formation	712	718
γ_{CH}	726	739
γ_{CH}	731	
γ_{CH}	744	751
γ_{CH+CC}	792	793
γ_{CH}	872	881
γ_{CH}	884	890
γ_{CH}	915	925
γ_{CH}	922	928
γ_{CH}	926	
Skeletal formation	972	962
γ_{CH}	978	971
β_{CH}	993	991
β_{CH}	1019	1020
β_{CH}	1021	1025
β_{CH}	1046	1054
β_{CH}	1049	1058
β_{CH}	1081	1087
β_{CH}	1109	1106
β_{CH}	1116	1114
β_{CH}	1118	1125
β_{CH}	1123	1134
β_{CH}	1148	1153
β_{CH}	1150	1155
β_{CH}	1157	1169
β_{CH}	1255	1246
β_{CH}	1256	1262
β_{CH}	1257	1269
Skeletal formation	1299	
β_{CH}	1413	1422
β_{CH}	1416	1424
β_{CH}	1433	1444
$\beta_{CH} + \nu_{CC}$	1570	
$\beta_{CH} + \nu_{CC}$	1576	1584
ν_{CH}	3091	
ν_{CH}	3096	3014
ν_{CH}	3112	3058
ν_{CH}	3119	3075

Note: γ represents out-of-plane bending vibration; ν represents stretching vibration; β stands for in-plane bending vibration.

Table S2. Lattice constants for Poly-BPH (0 K, 0 GPa).

	Poly-BPH
a (Å)	4.2879
b (Å)	4.0518
c (Å)	8.7744
α (°)	81.1247
β (°)	84.3549
γ (°)	85.3458
Cell Volume (Å^3)	149.550

Table S3. Atomic coordinates for Poly-BPH (0 K, 0 GPa).

Atom	x	y	z
H1	0.12928	0.76044	0.94504
H2	0.64977	0.93314	0.90437
H3	0.86486	1.02498	0.61907
C4	0.67149	0.47662	0.41040
C5	0.89966	0.43244	0.27651
C6	0.73494	0.27498	0.16425
C7	0.43910	0.18038	0.18653
C8	0.21037	0.22384	0.32517
C9	0.37438	0.38064	0.43279
H10	0.02371	0.32149	0.78222
H11	0.87072	0.23956	0.05496
H12	0.35023	0.06686	0.09563
H13	0.13514	-0.02498	0.38093
C14	0.32851	0.52338	0.58960
C15	0.10034	0.56756	0.72349
C16	0.26506	0.72502	0.83575
C17	0.56090	0.81962	0.81347
C18	0.78963	0.77616	0.67483
C19	0.62562	0.61936	0.56721
H20	0.97629	0.67851	0.21778

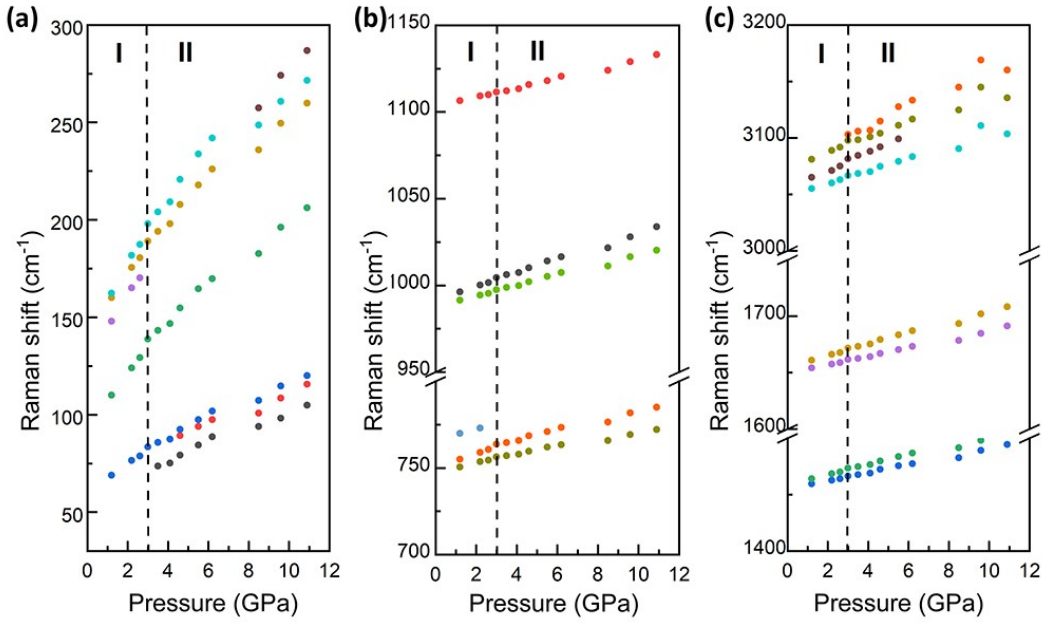

Figure S1. Pressure dependences of the Raman shifts (cm^{-1}) of biphenylene at room temperature. The dotted line represents the boundaries of different phases.

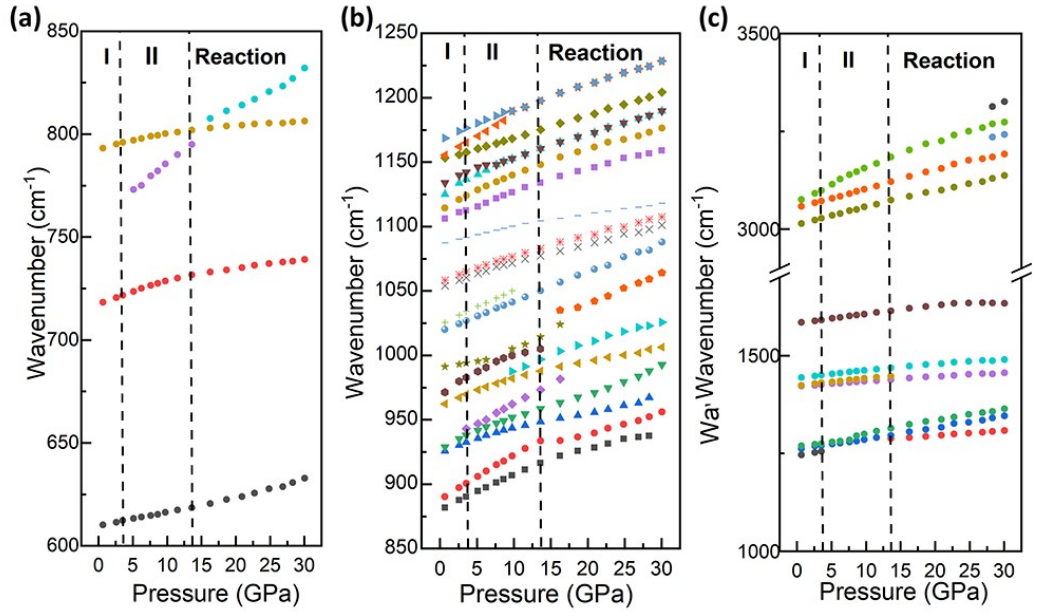

Figure S2. Pressure dependences of the Infrared active modes (cm^{-1}) of biphenylene at room temperature. The dotted line represents the boundaries of different phases.

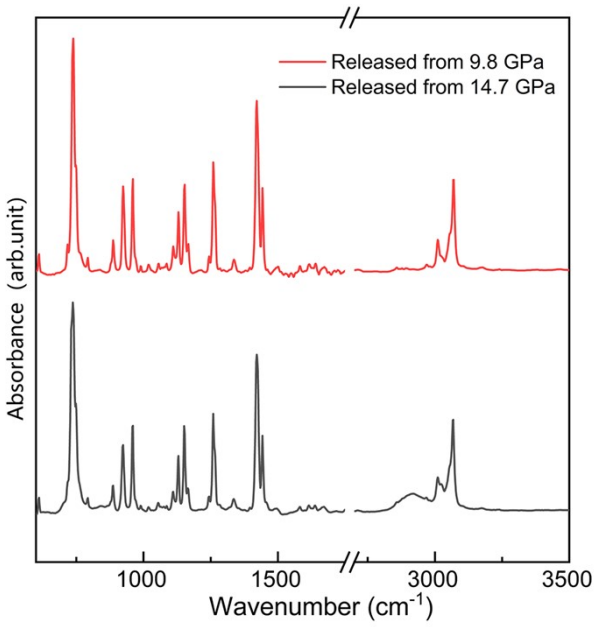

Figure S3. Infrared spectra of recovered biphenylene polymeric product from selected pressures.

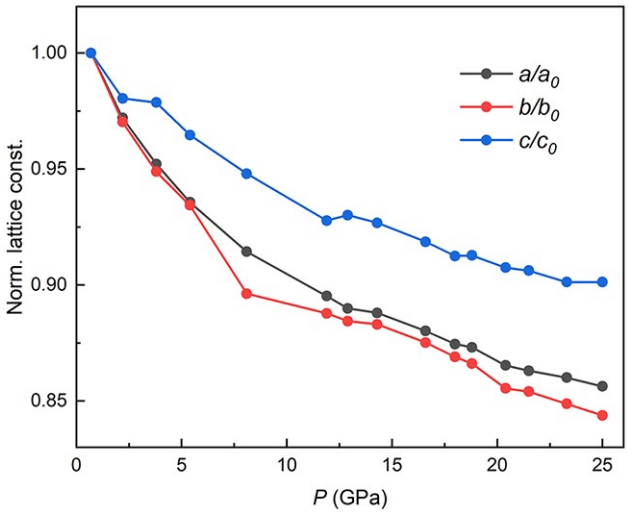

Figure S4. Evolution of corresponding compression ratio of lattice parameters from 0.9 to 25.0 GPa.

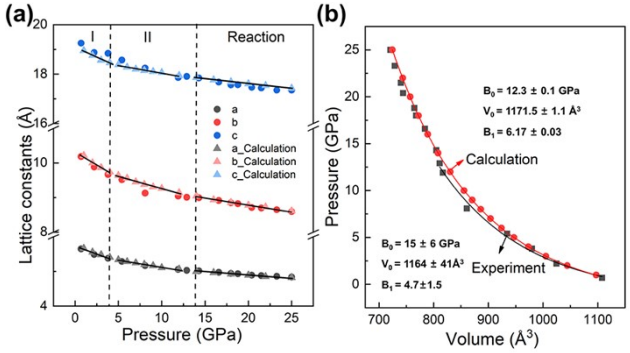

Figure S5. (a) Variations of lattice parameters during compression, as determined from experiments (solid circles) and DFT calculations (solid triangles). (b) Pressure dependence of the unit cell volume of biphenylene. The black squares represent experimental results and the red circles represent DFT calculations. The solid lines represent the fitting results of the 3rd order Birch−Murnaghan equation of state.

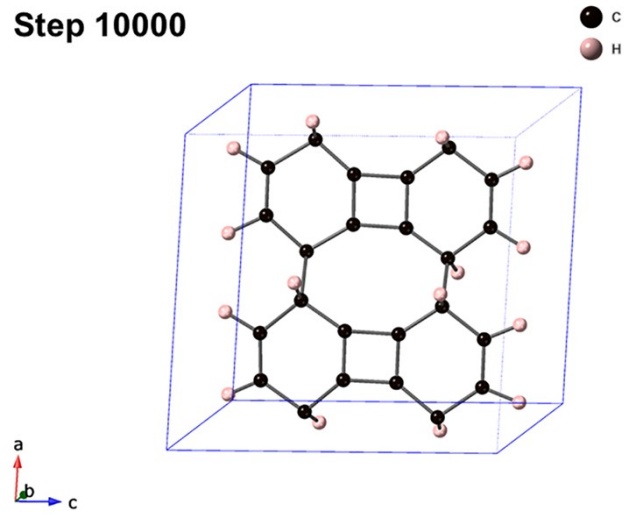

Figure S6. Crystal Structure of Poly-BPH at 300 K, simulated by molecular dynamic.

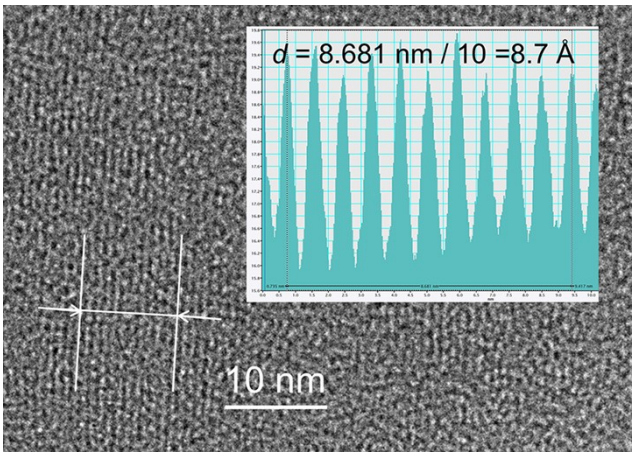

Figure S7. High-resolution transmission electron microscopy of poly-biphenylene.

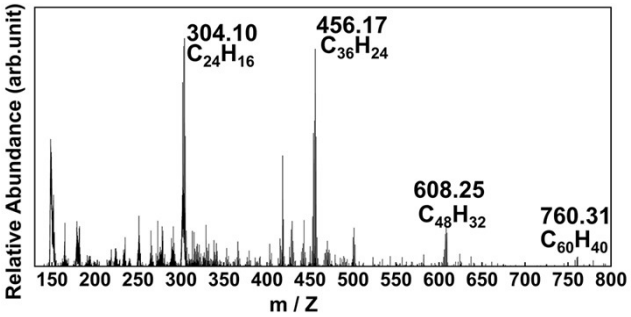

Figure S8. Matrix-assisted laser Desorption Ionization Time of Flight Mass Spectrometry (MALDI-TOF-MS) characterization of PE25 in the dichloromethane with the *trans*-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene] malononitrile (DCTB) as matrix. The signals at *m*/*z* = 250, and 500 are the peaks of DCTB clusters.