# SUPPLEMENTARY INFORMATION

## High-pressure and temperature dependence of the spontaneous resolution of enantiomers

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**Table S1**. Experimental parameters and crystal data of (±)-1,1'-binaphthyl.

| Formula | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ |
|---|---|---|---|---|---|---|
| Formula weight | 254.31 | 254.31 | 254.31 | 254.31 | 254.31 | 254.31 |
| Temperature (K) | **280(2) K** | **296(2)** | **296(2)** | **296(2)** | **296(2)** | **296(2)** |
| Pressure (GPa) | **0.001** | **0.001** | **0.05** | **0.10** | **0.30** | **0.45** |
| Wavelength (Å) | 0.71073 Å | 0.71073 Å | 0.71073 Å | 0.71073 Å | 0.71073 | 0.71073 Å |
| Crystal system | Monoclinic | Monoclinic | Monoclinic | Monoclinic | Monoclinic | Monoclinic |
| Space group | *C2/c* | *C2/c* | *C2/c* | *C2/c* | *C2/c* | *C2/c* |
| a (Å) | 21.107(2) | 21.1362(19) | 21.124(19) | 21.064(15) | 20.922(17) | 20.89(1) |
| b (Å) | 6.3354(5) | 6.3427(4) | 6.342(5) | 6.305(4) | 6.238(4) | 6.204(5) |
| c (Å) | 10.2009(9) | 10.2203(9) | 10.189(9) | 10.165(3) | 10.090(4) | 10.011(5) |
| β (°) | 105.090(13) | 105.098(12) | 105.08(1) | 105.11(2) | 105.08(3) | 105.14(4) |
| Volume (Å$^3$) | 1317.0(2) | 1322.84(19) | 1318.1(19) | 1303.4(13) | 1271.5(14) | 1252.4(14) |
| Calc. density (gcm$^{-3}$) | 1.283 | 1.277 | 1.282 | 1.296 | 1.329 | 1.349 |
| Z | 4 | 4 | 4 | 4 | 4 | 4 |
| Absorption coefficient (mm$^{-1}$) | 0.073 | 0.072 | 0.072 | 0.073 | 0.075 | 0.076 |
| F(000) | 536 | 536 | 536 | 536 | 536 | 536 |
| Crystal size (mm) | 0.20·0.10·0.08 | 0.20·0.10·0.08 | 0.40·0.20·0.05 | 0.40·0.18·0.05 | 0.35·0.15·0.05 | 0.30·0.18·0.05 |
| θ range for data collection (°) | 2.00 to 26.27 | 2.00 to 26.28 | 4.39 to 27.16 | 3.38 to 27.01 | 3.42 to 28.49 | 3.44 to 28.67 |
| Limiting indices: | | | | | | |
| *h* | -26/23 | -23/26 | -22/21 | -14/14 | -11/11 | -11/11 |
| *k* | -7/7 | -7/7 | -8/7 | -7/7 | -8/8 | -8/8 |
| *l* | -10/12 | -12/10 | -10/11 | -13/13 | -13/13 | -13/13 |
| Reflections collected/ unique | 4269/1307 | 4303/1309 | 3090/452 | 2811/441 | 3544/347 | 3522/486 |
| $R_{int}$ | 0.0274 | 0.0289 | 0.1493 | 0.1258 | 0.1100 | 0.1116 |
| $\theta_{max}$ (°)/Completeness (%) | 26.27/98.3 | 26.28/97.9 | 27.16/30.9 | 27.01/31.1 | 28.49/21.5 | 28.67/41.2 |
| Data/restraints/parameters | 1307/0/92 | 1309/0/92 | 452/60/88 | 441/60/91 | 347/60/91 | 486/0/122 |
| Goodness-of-fit on $F^2$ | 1.011 | 1.019 | 1.036 | 1.109 | 1.139 | 1.152 |
| Final $R_1$/w$R_2$ [$I>2\sigma_I$] | 0.0425/0.1152 | 0.0436/0.1226 | 0.0869/0.1499 | 0.0684/0.1010 | 0.0617/0.1503 | 0.0702/0.1115 |
| $R_1$/w$R_2$ indices (all data) | 0.0550/0.1266 | 0.0568/0.1352 | 0.1086/0.1285 | 0.0939/0.1645 | 0.1119/0.1654 | 0.1174/0.1462 |
| Largest diff. peak/hole (e.Å$^{-3}$) | 0.143/-0.130 | 0.134/-0.130 | 0.102/-0.098 | 0.128/-0.158 | 0.099/-0.103 | 0.165/-0.120 |

**Table S1 (continued)**. Experimental parameters and crystal data of (±)-1,1'-binaphthyl.

| Formula | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ |
|---|---|---|---|---|---|---|
| Formula weight | 254.31 | 254.31 | 254.31 | 254.31 | 254.31 | 254.31 |
| Temperature (K) | **296(2)** | **296(2)** | **296(2)** | **296(2)** | **296(2)** | **296(2)** |
| Pressure (GPa) | **0.55** | **0.70** | **1.16** | **1.29** | **2.21** | **2.97** |
| Wavelength (Å) | 0.71073 Å | 0.71073 Å | 0.71073 Å | 0.71073 Å | 0.71073 | 0.71073 Å |
| Crystal system | Monoclinic | Monoclinic | Monoclinic | Monoclinic | Monoclinic | Monoclinic |
| Space group | *C2/c* | *C2/c* | *C2/c* | *C2/c* | *C2/c* | *C2/c* |
| a (Å) | 20.809(16) | 20.770(5) | 20.584(13) | 20.575(10) | 20.41(2) | 20.32(1) |
| b (Å) | 6.185(2) | 6.1526(14) | 6.058(4) | 6.0390(9) | 5.934(3) | 5.888(2) |
| c (Å) | 10.044(4) | 9.991(1) | 9.874(5) | 9.8506(15) | 9.683(3) | 9.592(7) |
| β (°) | 105.22(1) | 105.30(2) | 105.24(2) | 105.34(4) | 105.49(3) | 105.50(2) |
| Volume ($Å^3$) | 1247.2(12) | 1231.5(4) | 1188.0(12) | 1180.4(6) | 1130.4(14) | 1105.9(10) |
| Calc. density ($gcm^{-3}$) | 1.354 | 1.371 | 1.422 | 1.431 | 1.494 | 1.527 |
| Z | 4 | 4 | 4 | 4 | 4 | 4 |
| Absorption coefficient ($mm^{-1}$) | 0.077 | 0.078 | 0.080 | 0.081 | 0.084 | 0.086 |
| F(000) | 536 | 536 | 536 | 536 | 536 | 536 |
| Crystal size (mm) | 0.40·0.20·0.05 | 0.35·0.18·0.05 | 0.40·0.20·0.05 | 0.35·0.16·0.05 | 0.40·0.20·0.05 | 0.40·0.20·0.05 |
| θ range for data collection (°) | 3.45 to 28.15 | 3.92 to 28.31 | 4.23 to 26.72 | 3.53 to 28.22 | 3.59 to 28.39 | 4.09 to 26.85 |
| Limiting indices: | | | | | | |
| *h* | -6/6 | -8/8 | -24/24 | -8/8 | -7/7 | -9/9 |
| *k* | -8/8 | -8/7 | -5/5 | -7/7 | -7/7 | -7/7 |
| *l* | -12/12 | -12/12 | -11/11 | -12/12 | -11/11 | -11/12 |
| Reflections collected/ unique | 3491/378 | 1863/532 | 2370/490 | 3492/420 | 3300/356 | 2663/357 |
| $R_{int}$ | 0.1081 | 0.1328 | 0.1781 | 0.1067 | 0.1157 | 0.1727 |
| $\theta_{max}$ (°)/Completeness (%) | 28.15/24.8 | 28.31/34.8 | 26.72/38.8 | 28.22/28.8 | 28.39/25.2 | 26.85/29.8 |
| Data/restraints/parameters | 378/60/92 | 532/60/91 | 490/60/91 | 420/60/92 | 356/60/92 | 357/60/80 |
| Goodness-of-fit on $F^2$ | 1.071 | 1.052 | 1.124 | 1.082 | 1.068 | 1.152 |
| Final $R_1$/w$R_2$ [$I>2\sigma_I$] | 0.0665/0.1411 | 0.0889/0.1195 | 0.1158/0.2127 | 0.0710/0.1696 | 0.0943/0.1290 | 0.0857/0.1899 |
| $R_1$/w$R_2$ indices (all data) | 0.1963/0.2129 | 0.0986/0.1863 | 0.1814/0.2202 | 0.1078/0.1841 | 0.1157/0.1326 | 0.1416/0.2088 |
| Largest diff. peak/hole ($e.Å^{-3}$) | 0.173/-0.153 | 0.133/-0.157 | 0.384/-0.341 | 0.189/-0.190 | 0.215/-0.148 | 0.278/-0.288 |

**Table S2**. Experimental parameters and crystal data of (-)-1,1'-binaphthyl.

| Formula | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ | $C_{20}H_{14}$ |
|---|---|---|---|---|---|---|---|---|
| Formula weight | 254.31 | 254.31 | 254.31 | 254.31 | 254.31 | 254.31 | 254.31 | 254.31 |
| Temperature (K) | **100(2)** | **150(2)** | **200(2)** | **250(2)** | **296(2)** | **296(2)** | **296(2)** | **296(2)** |
| Pressure (GPa) | **0.001** | **0.001** | **0.001** | **0.001** | **0.001** | **1.40** | **2.37** | **3.14** |
| Wavelength (Å) | 0.71073 Å | 0.71073 Å | 0.71073 Å | 0.71073 Å | 0.71073 | 0.71073 Å | 0.71073 Å | 0.71073 Å |
| Crystal system | Tetragonal | Tetragonal | Tetragonal | Tetragonal | Tetragonal | Tetragonal | Tetragonal | Tetragonal |
| Space group | $P4_12_12$ | $P4_12_12$ | $P4_12_12$ | $P4_12_12$ | $P4_12_12$ | $P4_12_12$ | $P4_12_12$ | $P4_12_12$ |
| a (Å) | 7.0872(3) | 7.1071(2) | 7.1316(2) | 7.1562(4) | 7.2063(2) | 6.8496(4) | 6.7514(15) | 6.6809(5) |
| b (Å) | 7.0872(3) | 7.1071(2) | 7.1316(2) | 7.1562(4) | 7.2063(2) | 6.8496(4) | 6.7514(15) | 6.6809(5) |
| c (Å) | 27.477(3) | 27.466(2) | 27.467(2) | 27.473(2) | 27.5057(14) | 26.691(3) | 26.507(10) | 26.433(3) |
| Volume ($Å^3$) | 1380.13(19) | 1387.33(13) | 1396.96(13) | 1406.93(19) | 1428.39(11) | 1252.3(2) | 1208.2(6) | 1179.84(19) |
| Calc. density ($gcm^{-3}$) | 1.224 | 1.218 | 1.209 | 1.201 | 1.183 | 1.349 | 1.398 | 1.432 |
| Z | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 |
| Absorption coefficient ($mm^{-1}$) | 0.069 | 0.069 | 0.068 | 0.068 | 0.067 | 0.076 | 0.079 | 0.081 |
| F(000) | 536 | 536 | 536 | 536 | 536 | 536 | 536 | 536 |
| Crystal size (mm) | 0.20·0.10·0.03 | 0.20·0.10·0.03 | 0.20·0.10·0.03 | 0.20·0.10·0.03 | 0.18·0.09·0.05 | 0.35·0.20·0.03 | 0.35·0.20·0.03 | 0.35·0.20·0.03 |
| θ range for data collection (°) | 2.97 to 29.11 | 2.96 to 29.12 | 2.95 to 29.09 | 2.94 to 29.03 | 3.19 to 26.48 | 3.34 to 28.58 | 3.11 to 27.78 | 3.42 to 28.83 |
| Limiting indices: | | | | | | | | |
| *h* | -9/9 | -9/9 | -9/9 | -9/9 | -9/8 | -8/8 | -3/3 | -8/8 |
| *k* | -9/9 | -9/9 | -9/9 | -9/9 | -8/8 | -4/4 | -8/8 | -3/3 |
| *l* | -37/37 | -37/37 | -37/37 | -37/37 | -33/33 | -33/33 | -30/29 | -33/34 |
| Reflections collected/ unique | 25896/1787 | 26030/1799 | 26194/1809 | 26352/1829 | 23469/1454 | 7536/1145 | 963/564 | 6986/1084 |
| $R_{int}$ | 0.0840 | 0.0928 | 0.1052 | 0.1172 | 0.0705 | 0.2240 | 0.1185 | 0.2095 |
| $\theta_{max}$ (°)/Completeness (%) | 29.11/97.2 | 29.12/97.3 | 29.09/97.7 | 29.03/98.6 | 26.48/99.2 | 28.58/71.9 | 27.78/41.2 | 28.83/70.7 |
| Data/restraints/parameters | 1787/0/92 | 1799/0/92 | 1809/0/92 | 1829/0/92 | 1454/0/92 | 1145/0/91 | 564/60/92 | 1084/60/92 |
| Goodness-of-fit on $F^2$ | 1.005 | 1.025 | 1.020 | 1.001 | 1.045 | 1.053 | 1.146 | 1.123 |
| Final $R_1$/w$R_2$ [$I>2\sigma_I$] | 0.0696/0.0925 | 0.0724/0.0958 | 0.0765/0.1027 | 0.0761/0.1365 | 0.0513/0.0850 | 0.1095/0.1673 | 0.0995/0.1387 | 0.1017/0.1461 |
| $R_1$/w$R_2$ indices (all data) | 0.0781/0.1121 | 0.0951/0.1191 | 0.1192/0.1301 | 0.0976/0.1749 | 0.0969/0.0960 | 0.1200/0.1692 | 0.1070/0.1477 | 0.1161/0.1471 |
| Largest diff. peak/hole ($e.Å^{-3}$) | 0.170/-0.144 | 0.140/-0.162 | 0.143/-0.143 | 0.126/-0.155 | 0.081/-0.083 | 0.404/-0.497 | 0.270/-0.308 | 0.405/-0.355 |

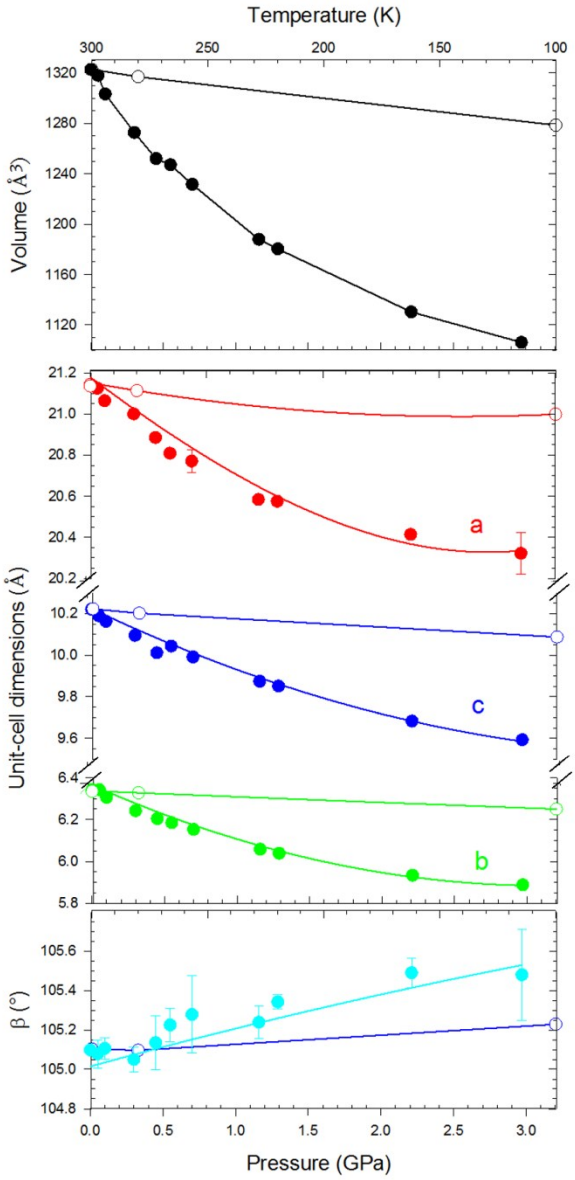


**Figure S1**. Volume, unit-cell parameters and the monoclinic β angle of (±)-1,1'-binaphthyl plotted as a function of pressure (full circles) and temperature (open circles). The 100 K (*RS*)-11'BN data after Ref. S1.

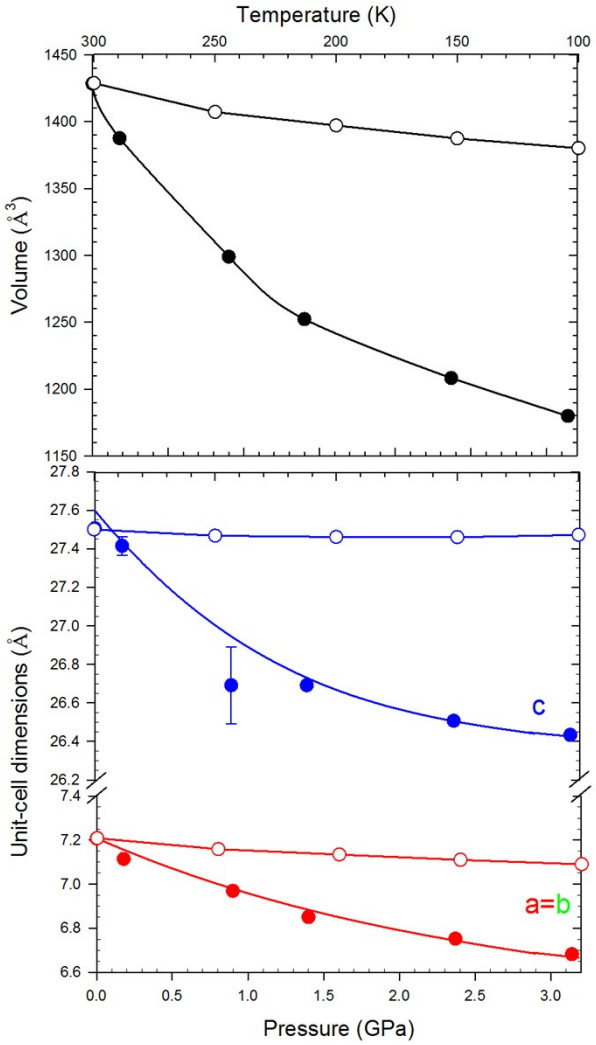


**Figure S2.** Unit-cell parameters and volume of (-)-1,1'-binaphthyl plotted as a function of pressure (full circles) and temperature (open circles).

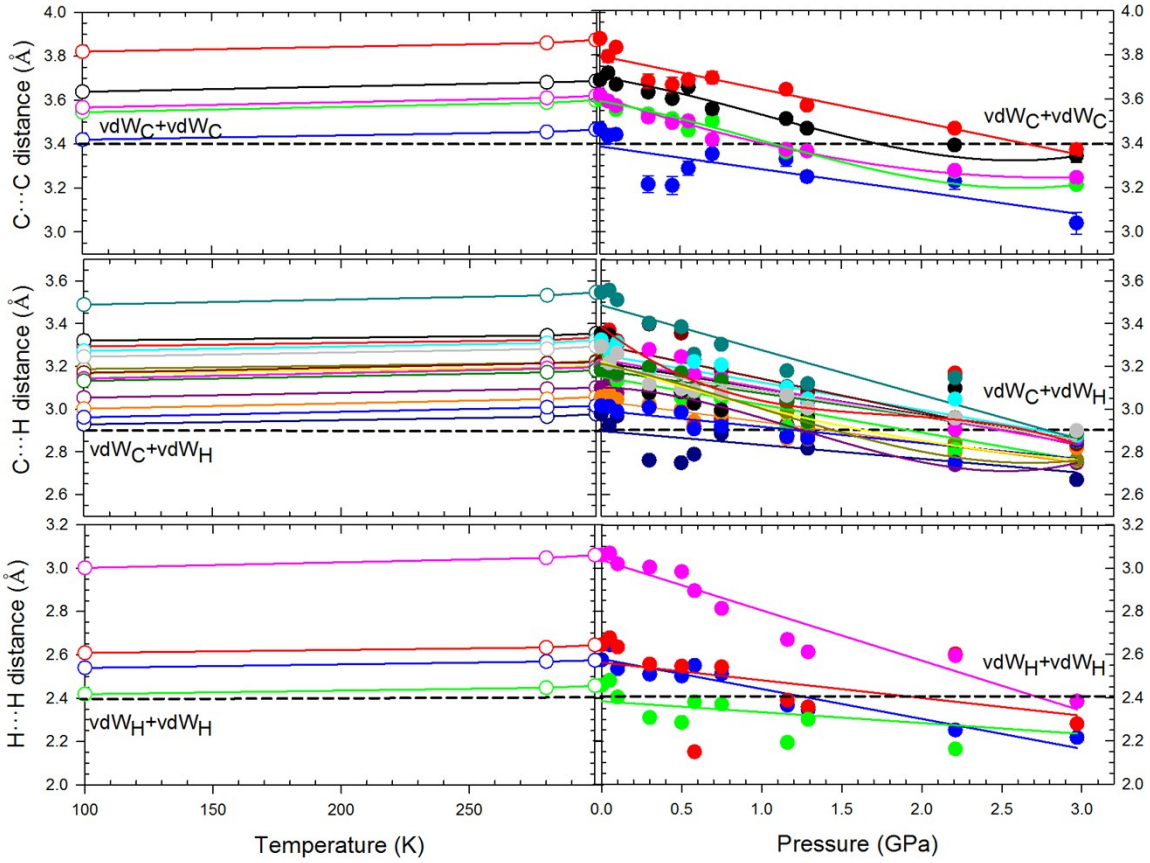


**Figure S3**. Pressure and temperature dependence of shortest intermolecular contacts of (±)-11'-BN. The dashed lines indicate the sums of van der Waals radii[2] (vdW) of atoms H···H, H···C and C···C as indicated by the subscripts.

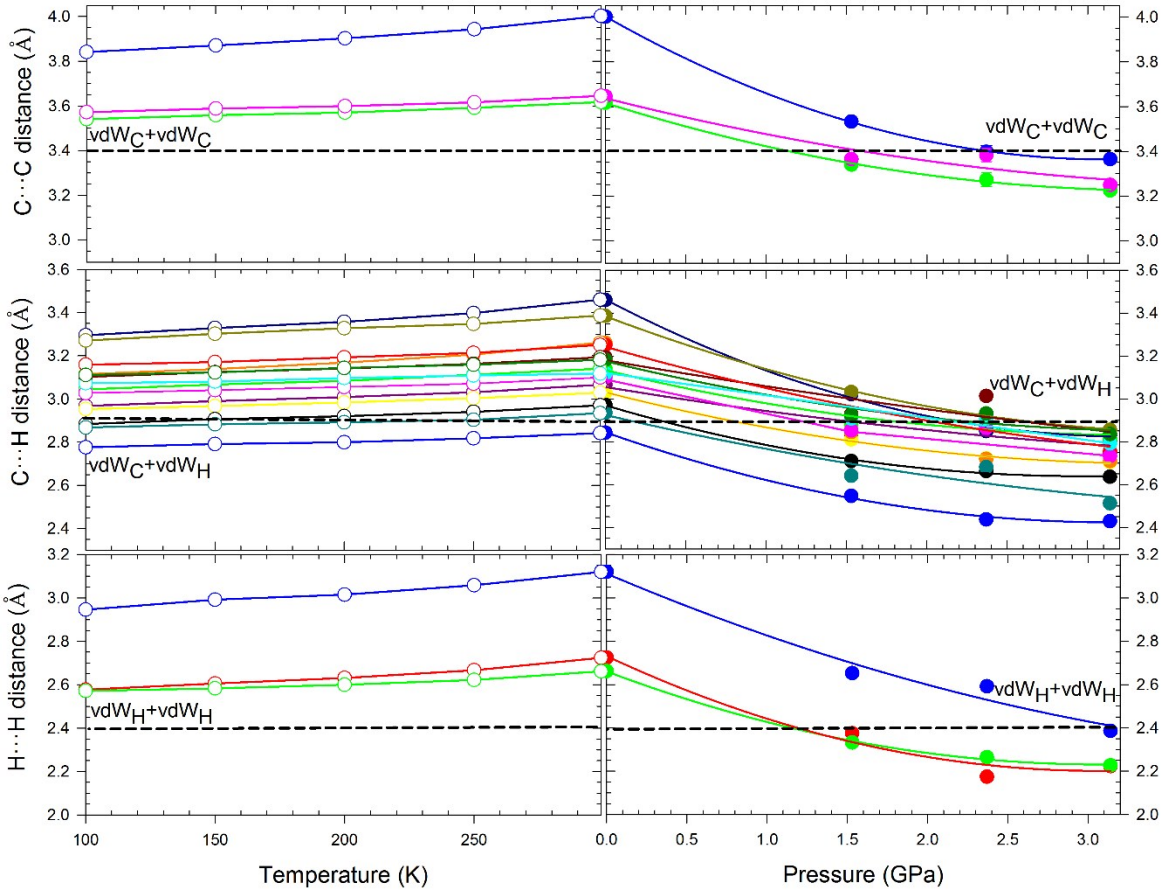


**Figure S4**. Pressure and temperature dependence of shortest intermolecular contacts of (-)-11'BN. The dashed lines indicate the sums of van der Waals radii[2] (vdW) of atoms H···H, H···C and C···C as indicated by the subscripts.

## References

S1. Stibrany, R. T.; Potenza, J. A. *Private Communication* (2006)

S2. Bondi, A. Van der Waals volumes and radii. *J. Phys. Chem.* **68**, 441–451 (1964).