Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

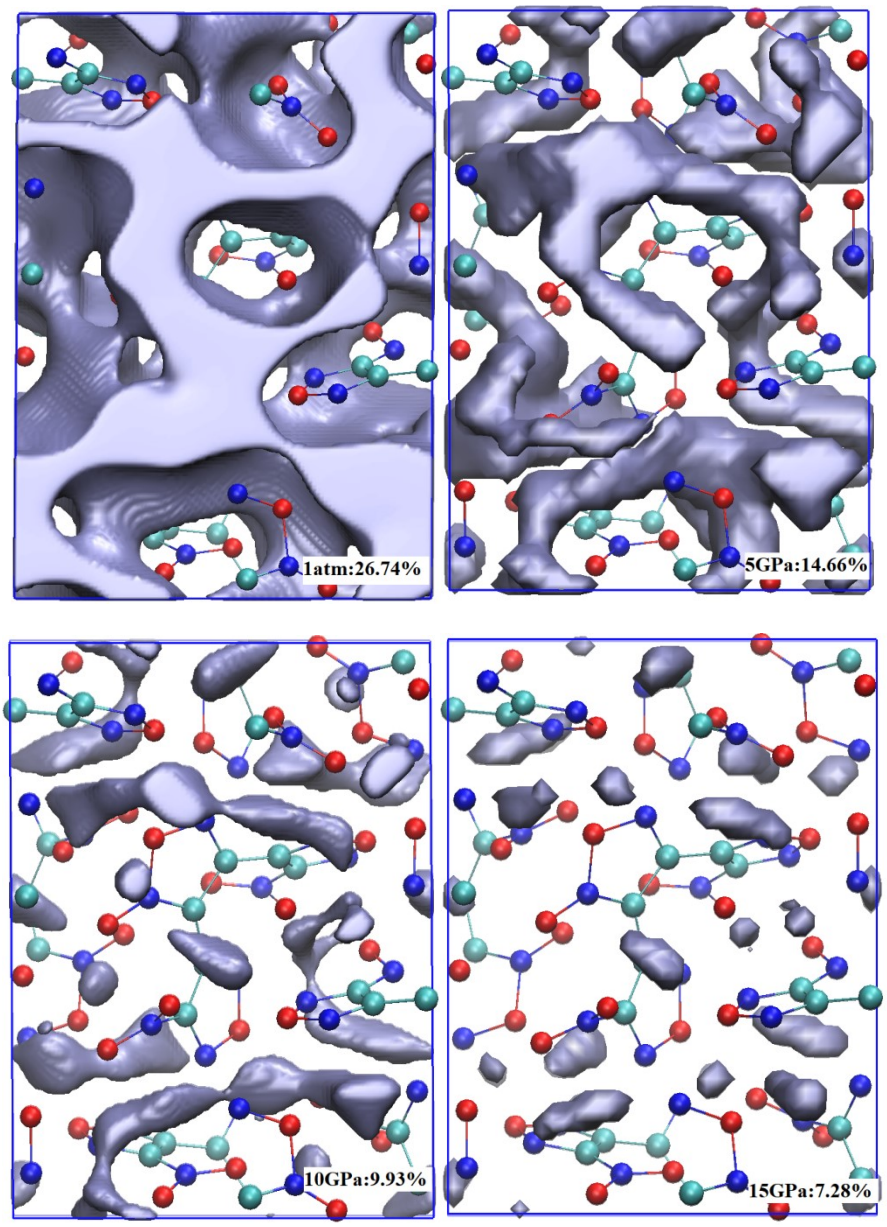
Supporting Information

Infrared Spectra and Electronic Structural changes of DNTF under High Pressure: Experimental and Theoretical Study

Table S1. The vibration energy distribution of DNTF at ambient pressure.

Theo. Freq. (cm^{-1})	Exp. Freq. (cm^{-1})	Vibration Energy Distribution
959	963	N-O stretching vibration in furoxan rings
1003	1002	N-O stretching vibration in furoxan rings
1040	1042	N-C stretching vibration in furazan rings
1176	1176	C-C bending vibration and N-O stretching vibration in furoxan rings
1290	1285	C-C stretching vibration in furazan rings and NO_2 symmetric stretching vibration
1322	1319	NO_2 symmetric stretching vibration
1362	1355	C-C stretching vibration in furazan rings
1521	1519	NO_2 asymmetric stretching vibration and little C-C stretching vibration
1555	1564	C-C stretching vibration between furazan ring and furoxan ring
	1587	N-O_c stretching vibration
1640	1641	N-O_c stretching vibration

Note: O_c represents the coordinated oxygen atom.


1atm:26.74%
5GPa:14.66%
10GPa:9.93%
15GPa:7.28%

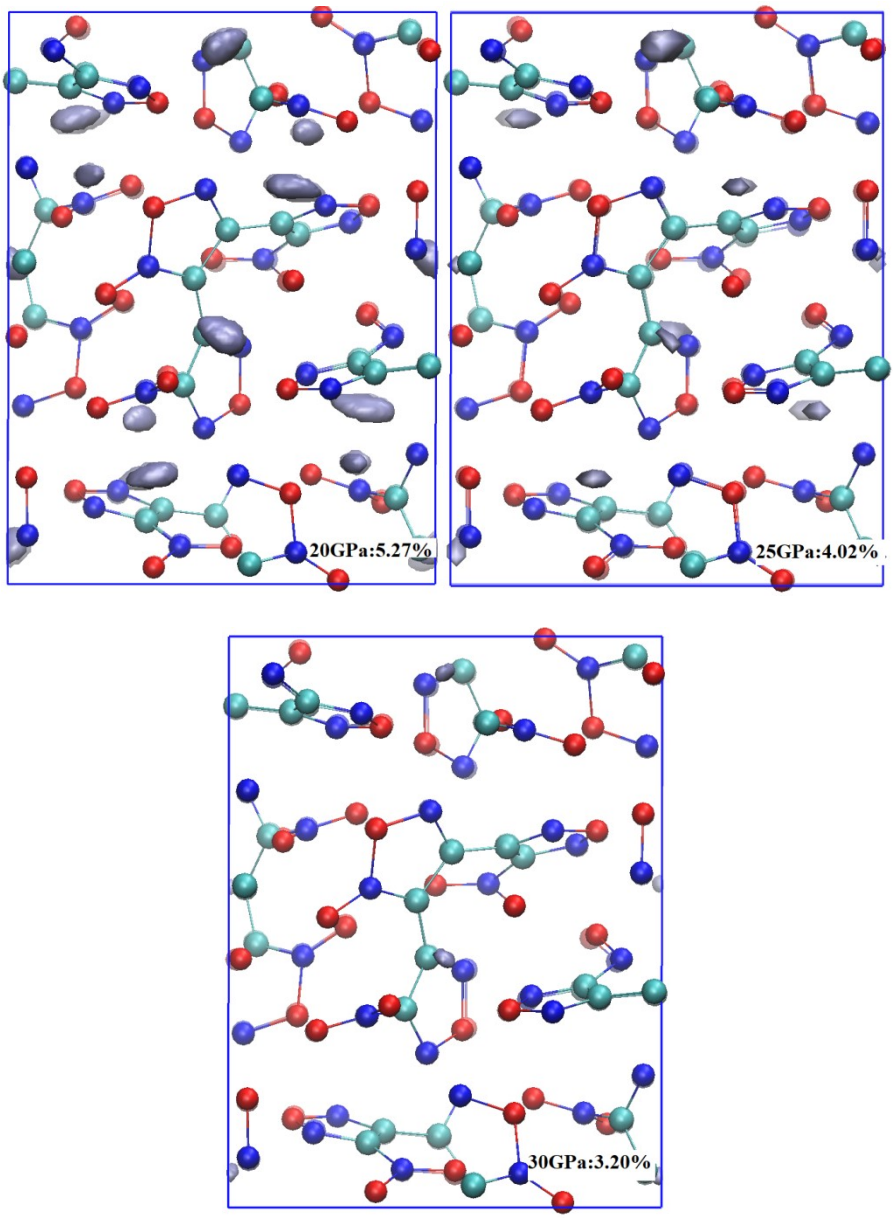


Figure S1. The evolution of free region in DNTF crystal at different pressure, and the iceblue isosurface represents the 0.03 a.u. region.