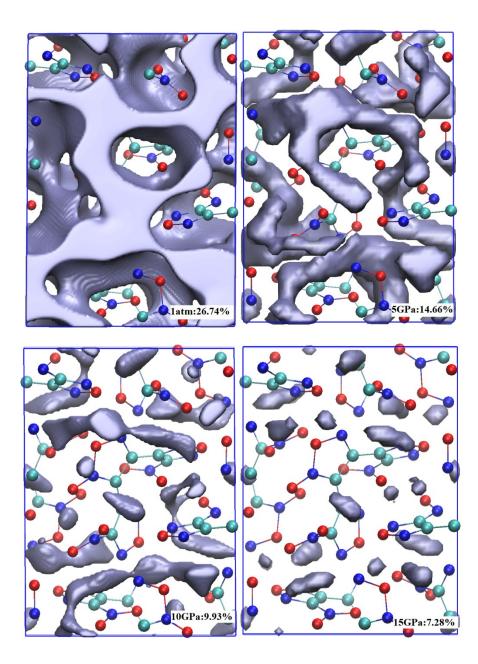
Supporting Information

Infrared Spectra and Electronic Structural changes of DNTF under

High Pressure: Experimental and Theoretical Study

1176 1176 vibration in furoxan rings 1290 1285 C-C stretching vibration in furazan rings an NO2 symmetric stretching vibration 1322 1319 NO2 symmetric stretching vibration 1362 1355 C-C stretching vibration in furazan rings 1521 1519 NO2 asymmetric stretching vibration and litt 1555 1564 C-C stretching vibration between furazan ring 1540 1587 N-Oc stretching vibration 1640 1641 N-Oc stretching vibration				
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1176 1176 vibration in furoxan rings 1290 1285 C-C stretching vibration in furazan rings an NO2 symmetric stretching vibration 1322 1319 NO2 symmetric stretching vibration 1362 1355 C-C stretching vibration in furazan rings 1521 1519 NO2 asymmetric stretching vibration and litt 1555 1564 C-C stretching vibration between furazan ring 1540 1587 N-Oc stretching vibration 1640 1641 N-Oc stretching vibration		1040	1042	N-C stretching vibration in furazan rings
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12901285NO2 symmetric stretching vibration13221319NO2 symmetric stretching vibration13621355C-C stretching vibration in furazan rings15211519NO2 asymmetric stretching vibration and litt15551564C-C stretching vibration between furazan ring1587N-Oc stretching vibration16401641N-Oc stretching vibration				vibration in furoxan rings
NO2 symmetric stretching vibration13221319NO2 symmetric stretching vibration13621355C-C stretching vibration in furazan rings15211519NO2 asymmetric stretching vibration and litt15551564C-C stretching vibration between furazan ring15551564C-C stretching vibration between furazan ring1587N-Oc stretching vibration16401641N-Oc stretching vibration		1290	1285	C-C stretching vibration in furazan rings and
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C-C stretching vibration15551564C-C stretching vibration between furazan ring and furoxan ring1587N-Oc stretching vibration16401641N-Oc stretching vibration		1521	1519	NO ₂ asymmetric stretching vibration and little
1555 1564 and furoxan ring 1587 N-O _c stretching vibration 1640 1641 N-O _c stretching vibration				C-C stretching vibration
and furoxan ring 1587 1640 1641 N-Oc stretching vibration		1555	1564	C-C stretching vibration between furazan ring
1640 1641 N-Oc stretching vibration				and furoxan ring
			1587	N-O _c stretching vibration
Note: O _c represents the coordinated oxygen atom.	1640		1641	N-O _c stretching vibration
	Note:	O _c	represents the	coordinated oxygen atom.

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



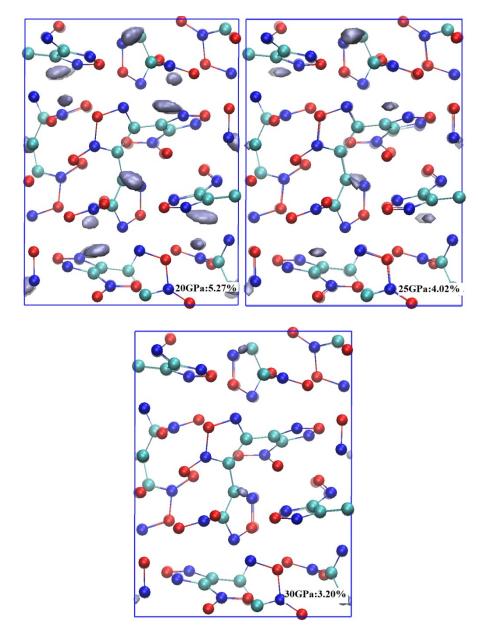


Figure S1. The evolution of free region in DNTF crystal at different pressure, and the iceblue isosurface represents the 0.03 a.u. region.