Supporting Materials

Effect of Pressure Gradient and New Phases for 1, 3, 5-trinitrohexahydro-s-triazine(RDX) under High Pressure

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Figure S1 Raman spectra of RDX under high pressure below 5 GPa with argon as PTM.

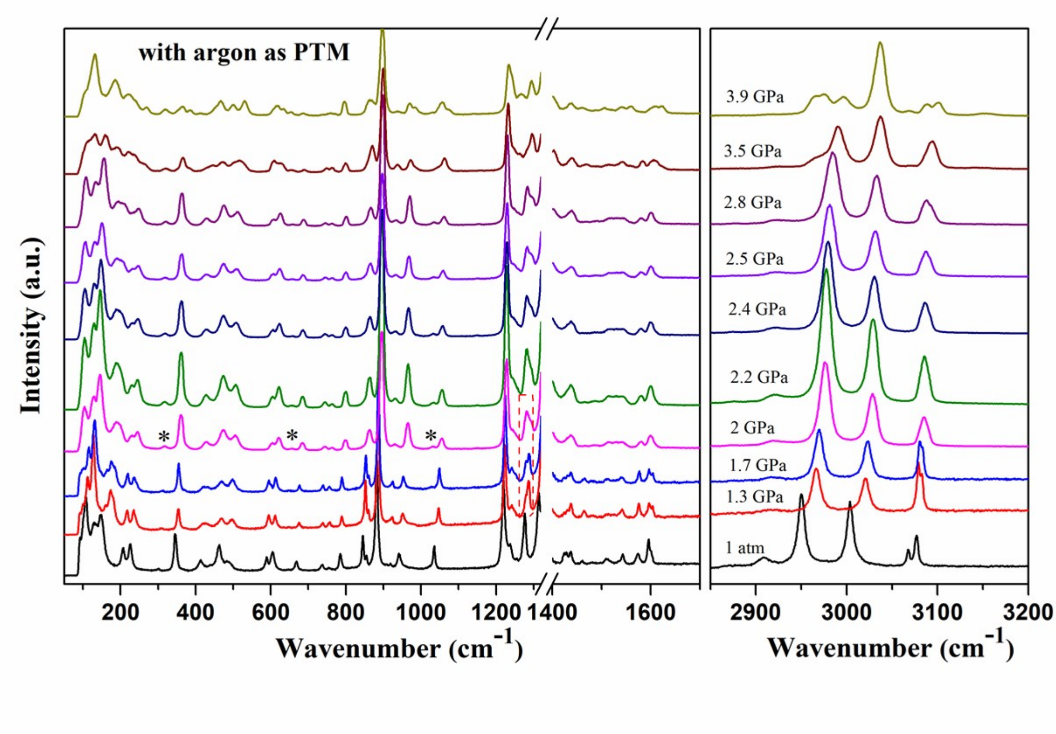


Figure S2 The different conformations of RDX [3]. The orientations of the nitro-groups can be distinguished by the angle between the plane of the C-N-C and the corresponding N-N bond.

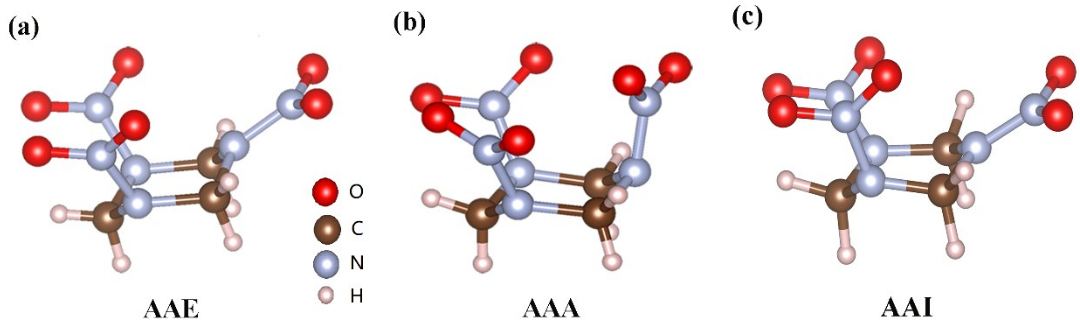
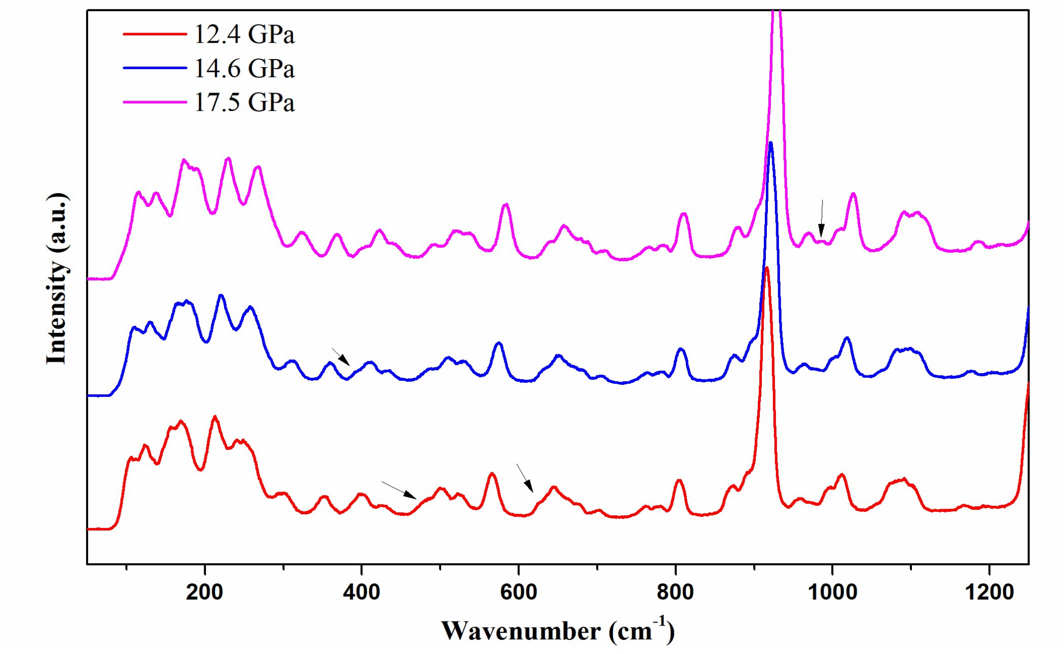


Figure S3 The enlarged spectra of RDX at 12.4 GPa, 14.6 GPa and 17.5 GPa.



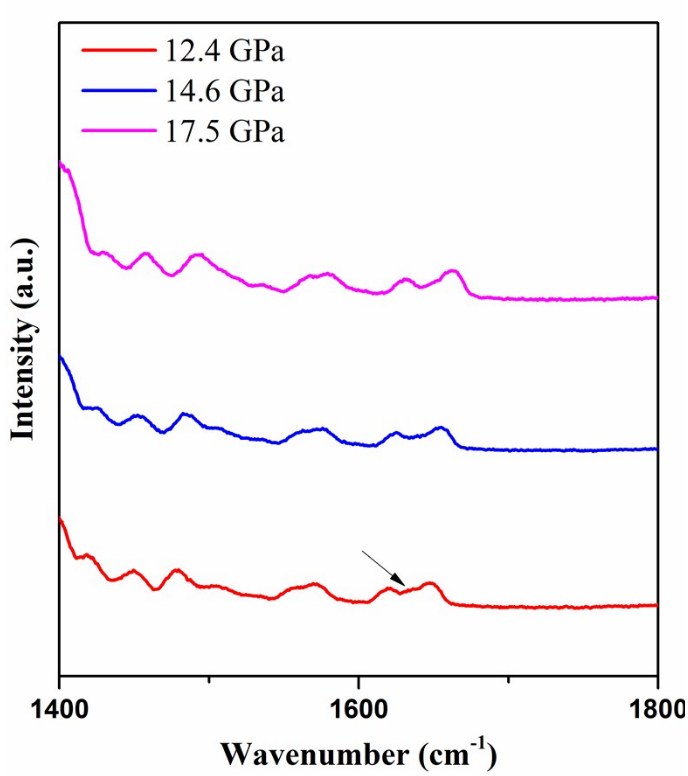


Figure S4 Raman spectra of RDX under high pressure below 5 GPa with silicon oil as PTM.

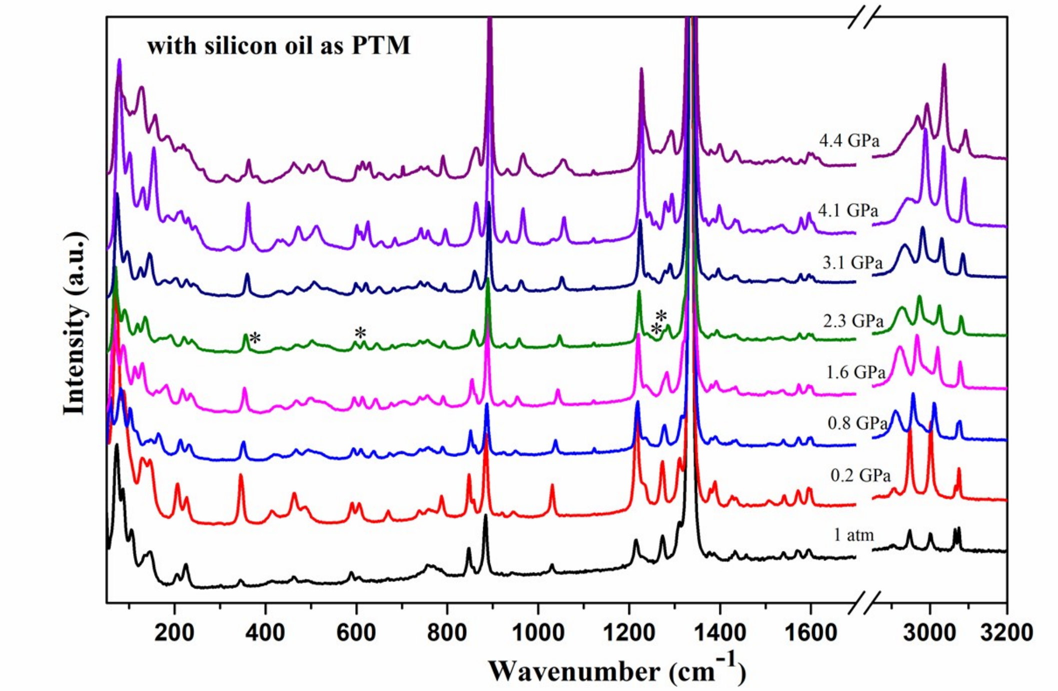


Figure S5 Raman spectra of RDX under high pressure below 5 GPa with 4:1 methanol-ethanol as PTM.

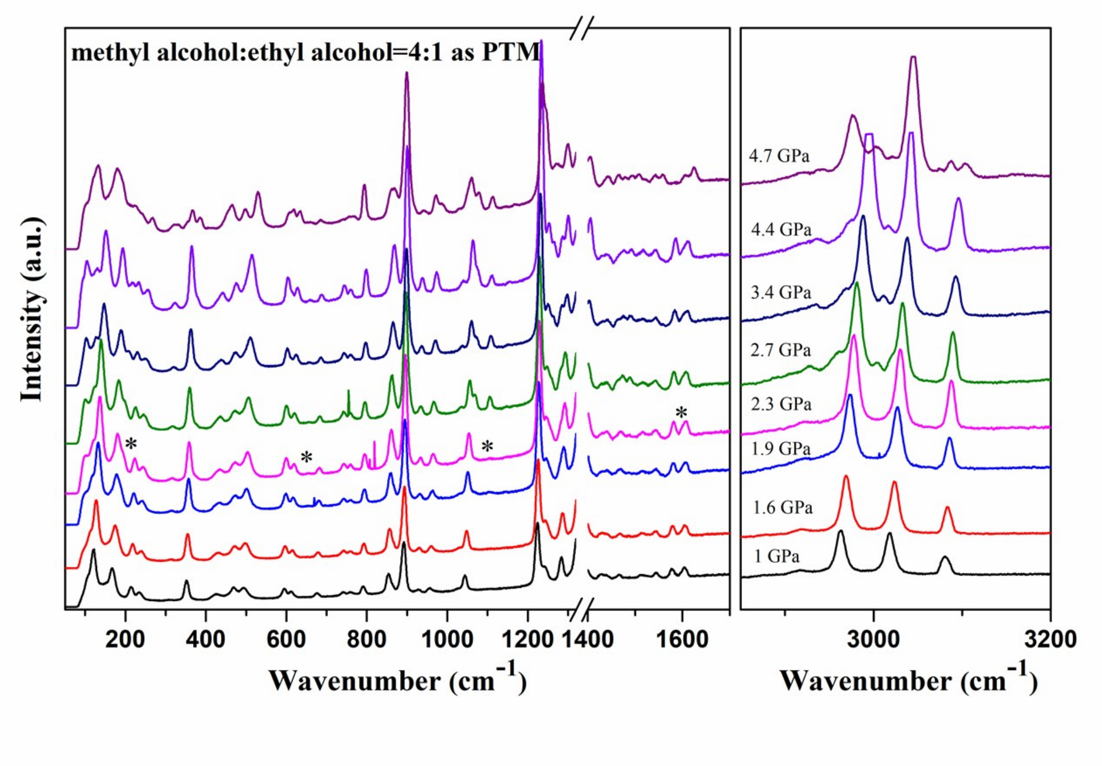


Figure S6 Raman spectra of RDX under high pressure below 5 GPa without PTM.

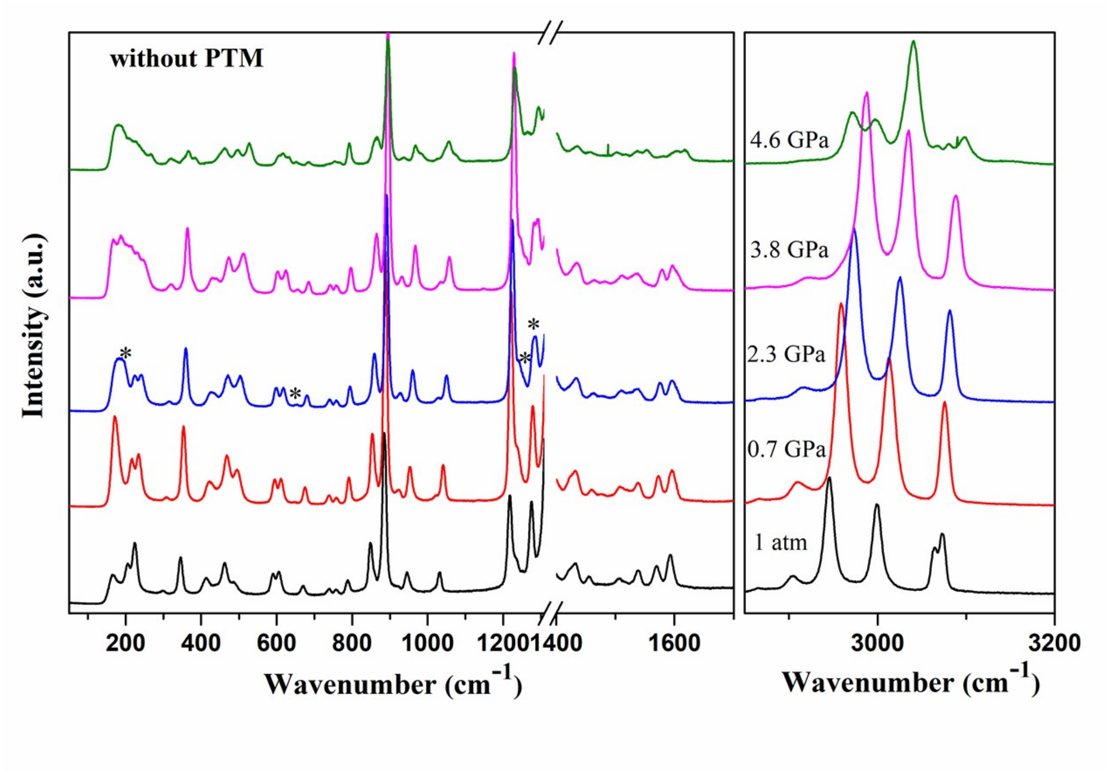


Figure S7 Raman spectra of RDX with non-hydrostatic compression without PTM.

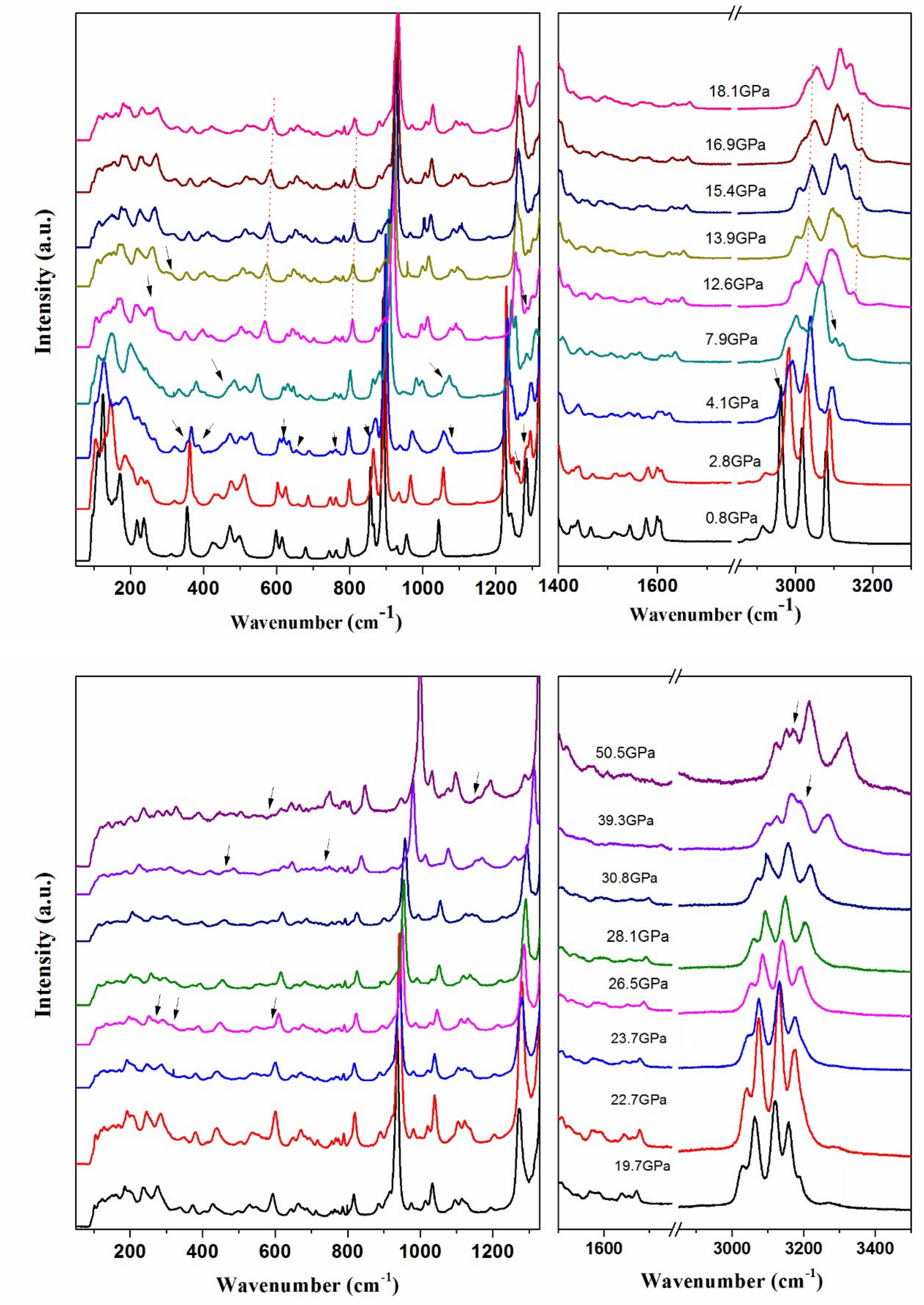


Figure S8 Raman shift of C-H stretching mode of RDX with different compression environment.

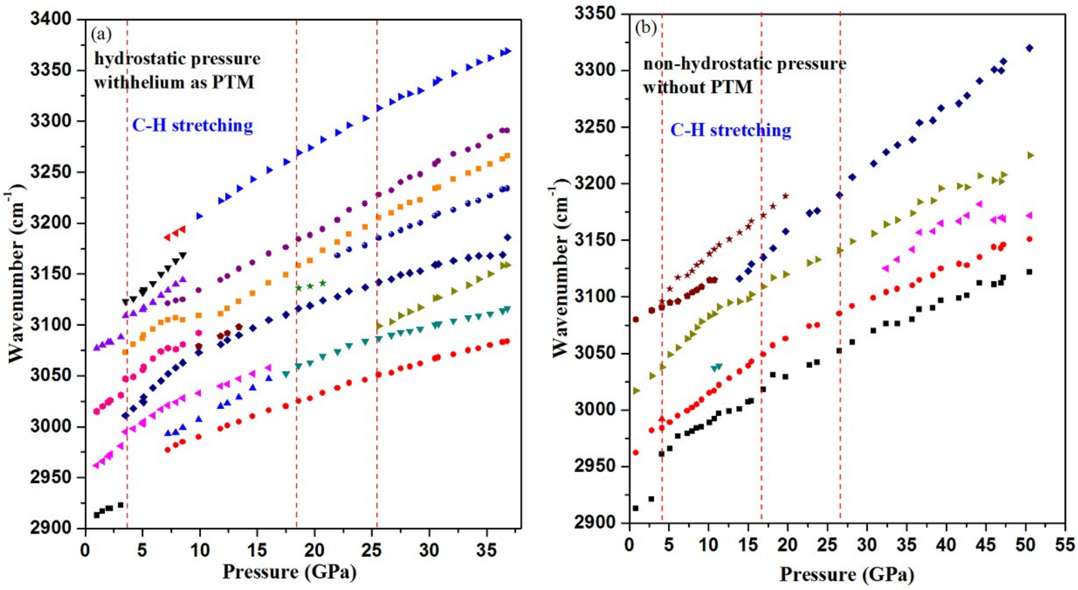


Figure S9 885 cm^{-1} breathing mode shifts of RDX with pressure up to 38 GPa, under hydrostatic condition with helium as PTM. (In the fitting equation, P is the pressure, ω means the Raman shift.)

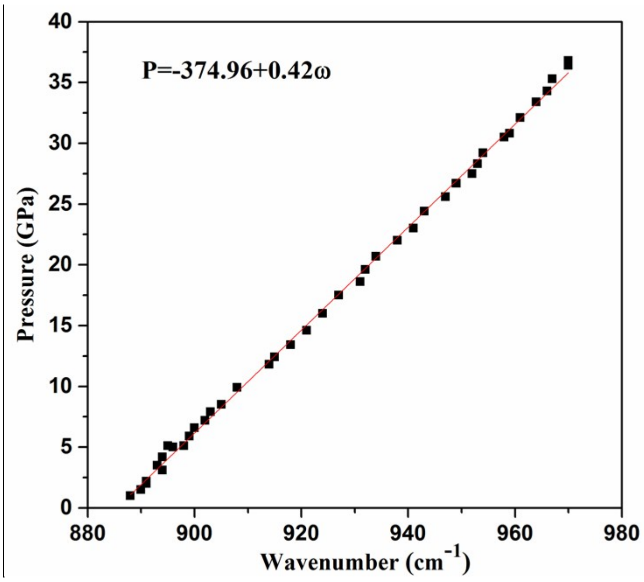


Figure S10 The pressure gradient in the sample chamber of DAC with silicon oil as PTM.

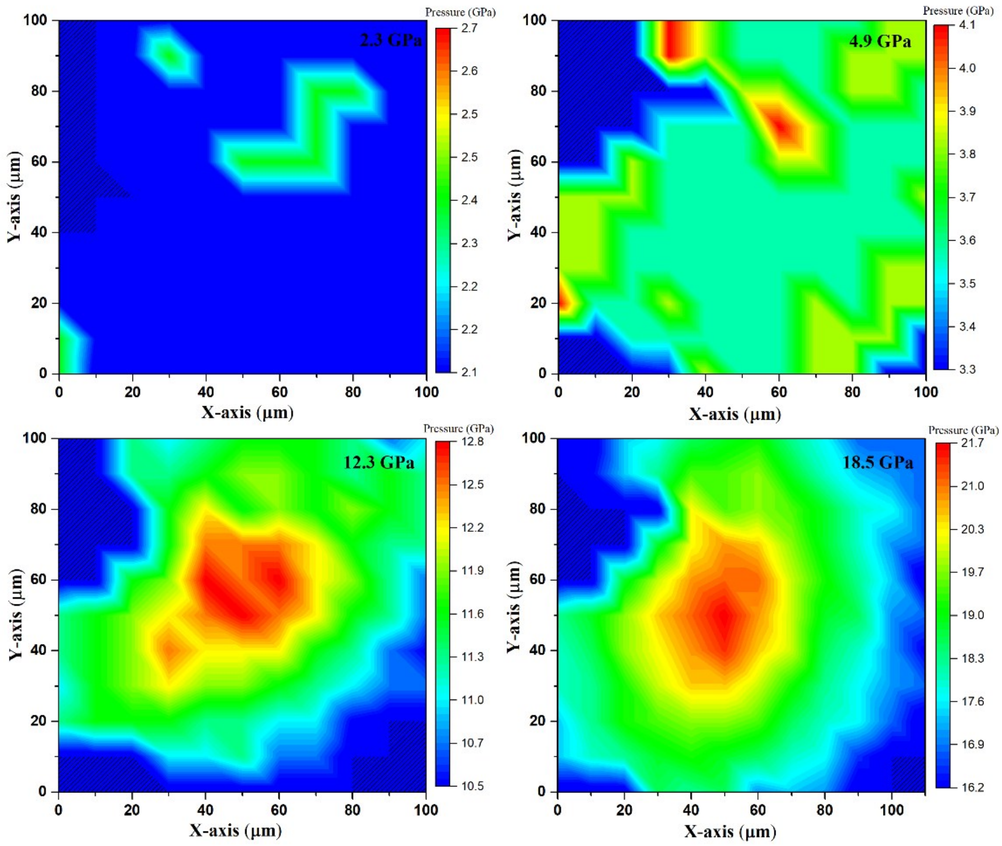


Table S1 Frequencies of Raman Modes and Infrared modes of RDX at different pressure

1 atm				high pressure			1 atm		
Raman (cm^{-1})				γ	δ	ζ	IR (cm^{-1})		
mode	this work	reference [2]	assign	3.5 GPa	17.5 GPa	30.5 GPa	this work	reference [14]	assign
					3260	3338			
					3176	3258			
				3126					
v1	3076	3076	CH st(ax)	3109			3075	3075	C-H st(ax)
v2	3066	3067	CH st(ax)			3234	3065	3065	C-H st(ax)
						3207			
				3081	3149				
v3	3000	3001	CH st(eq)	3047			3001	3001	C-H st(eq)
				3018	3110	3159			
						3126			
					3052	3100			
					3020	3067			
v4	2947	2949	CH st(ax)	2995			2947	2949	C-H st(ax)
v5	2904	2906	CH st(ax)				2913	2911	C-H st(ax)
v6	2869		CH st(eq)				2862		C-H st(eq)
				1616	1662	1699	1594	1593	O-N-O st(ax)
v7	1595	1595	O-N-O st(ax)	1609					
				1600	1631	1660			
						1607			
						1543			
v8	1572	1573	O-N-O st(ax)	1578			1573	1570	O-N-O st(eq)
				1564	1580				
v9	1540	1542	O-N-O st(eq)	1544	1567		1533	1539	O-N-O st(eq)
					1491	1510			
v12	1508	1508	CH_2 sci or comb	1517			1458	1458	CH_2 sci
v14	1458	1460	CH_2 sci						

v15	1434	1436	CH_2 sci	1440	1456	1484	1435	1436	CH_2 sci
							1422	1423	CH_2 (in plane and out of plane bending)
v18	1387	1388	CH_2 wag	1400	1430		1389	1388	CH_2 wag
v19	1377	1377	CH_2 tw				1351	1374	N-NO_2 (ax)st
v23	1310	1309	CH_2 tw,N-N st				1311	1311	N-NO_2 st
v24	1273	1273	CH_2 tw,N-N st(ax)				1269	1268	CH_2 twist+N-N st
v26	1232	1232	CH_2 tw or comb				1233	1234	N-C-N st
v27	1215	1215	N-C st	1229	1269	1295	1217	1218	N-C st
					1184	1232	1040	1039	N-C st
					1107	1148			
					1090	1134			
						1112			
					1025	1057			
v28	1030	1031	N-C st	1059			1018	1029	ring st
				1030					
v30	943	945	N-N st(eq)	962	1008		945	943	N-N st(eq)+ CH_2 twist+CH_2 rock
					987	1023			
v31	921	920	CH_2 r or comb	932	968	996	925	925	
							914	915	CH_2 bending
v32	885	885	C-N st	893	927	958	881	884	C-N st+CH_2 rock+N-N st

v33	857	858	C-N st	867	901		851	853	N-N st+NO_2 sci(ax)
					878	903	842	847	
v34	847	848	N-N st,NO_2 sci(ax)		810	823			
v35	784	788	C-N st,NO_2 sci	802	783	794	782	786	C-N st+NO_2 sci(eq)
							754		
v36	757	757	ring b,NO_2 sci,or comb	763			737	739	N-NO_2 unbrella (ax)
v37	739	742	N-NO_2 u(ax)or comb	740	764	775			
						755			
v38	669	670	ring b	681	708	730	670	669	ring b
				647	685	716			
v39	605	607	ring r	626			604	605	ring r
v40	590	590	ring b	611	656	688	587	588	ring b
					640	670			
v42	490	495	ring tw, NO_2 sci	523	583	621		486	ring twist+NO_2 rock(eq)
						590			
						566			
v43	462	464	ring b(fold), N-N st(eq)	494	537			463	ring bending (folding)+N-N st(ax)
v45	416	415	ring b(flattening)	439	520			414	ring bending (folding)
					491	523			
						490			
				404	441				
v47	346	347	ring tw	373	421	462		347	ring twist

					402	431		
					367	400		
					324	385		
						335		
					266	295		
v48	301	301	molecular st or overtone	323				
				248				
v49	224	226	ring rot				224	ring rotation +NO_2 rotation (all)
v50	205	207	N-NC(2) nmbrella(eq)				205	N-NC(2) unmbrella(eq)+ NO_2 rotation (ax)
v51	144	149	NO_2 tor	214				
v52	133	131	NO_2 tor	144	229	264		
					190	224		
					172	205		
v53	105	107	molecular b		137	165	106	molecular bend+NO_2 ratation
v54	86	90	NO_2 tor(ax)	104		137		
					115	112		

Abbreviations: st=stretch, tw=twist, r=rock, b=bend, u=umbrella, wag=wag, rot=rotation, sci=scissor,f=fold,tor=torsion, comb/OT=combination or overtone, ax=axial, eq=equatorial, skl=skeletal, def=deformation.