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High-pressure stability of 1,1-diamino-2,2-dinitroethene (FOX-7): H/D isotope effect



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ABSTRACT

H/D substitution was used to gain insight into the role of hydrogen bonding (HB) on the high-pressure stability of FOX-7. Raman measurements were performed on single crystals of deuterated FOX-7 (FOX-7-d₄) compressed to 40 GPa. Comparison of present and previously published results for FOX-7 revealed that deuteration: (i) does not affect chemical stability to 40 GPa, (ii) removes spectral changes observed at 2 GPa, (iii) does not affect the pressure onset for the 4.5 GPa phase transition, and (iv) lifts the vibrational modes coupling. This work demonstrates that HB contributes selectively to different aspects of the high-pressure stability of FOX-7.

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1. Introduction

1,1-Diamino-2,2-dinitroethene ([C₂(NH₂)₂(NO₂)₂], FOX-7 or DADNE) is a high explosive (HE) crystal with excellent performance and low initiation sensitivity [1–5]. Although its low sensitivity to impact and shock waves is of considerable interest, the microscopic factors governing this behavior are not well understood. To gain insight into this behavior several experimental [6–10] and theoretical [11–15] studies have been conducted to characterize the molecular response of FOX-7 at high pressures. In accord with its low sensitivity to initiation, it was recently shown that FOX-7 single crystals are chemically stable over a broad range of pressure [10]. However, a number of new vibrational features were observed in the Raman spectra. They were attributed to two polymorphic transformations at 2 and 4.5 GPa; also, the Raman data showed considerable modifications in the hydrogen bonding and a significant increase in vibrational modes coupling under high pressures. It was suggested that these processes may be responsible for the increased stability of FOX-7 at high pressures and, thus, its low sensitivity to shock initiation [10]. Because the ambient structure of FOX-7 is stabilized by the hydrogen bonds [2], it is reasonable to link these processes to their presence. Here we present results on deuterated FOX-7 (FOX-7-d₄) to examine this link, and to further the understanding the role of hydrogen bonding on the high-pressure stability of FOX-7.

It is well recognized that the H/D substitution in hydrogen bonded systems can affect the structure of the A–X···B bond (A = donor, X = H or D, and B = acceptor), e.g., [16–18]. This structural effect is also referred to as the geometric isotope effect (GIE), and is commonly associated with changes in the bond vibrations. The decrease of the zero-point vibrational energy (ZPVE) of a deuterated compound along with the anharmonicity of the bond potential leads to a shortening of the covalent A–D bond as compared to the A–H bond. The covalent bond length shortening due to deuteration is usually accompanied by the lengthening of the donor–acceptor (A···B) distance, known as the Ubbelohde effect [19]. Thus, the proton–deuteron substitution by modifying the hydrogen bond (HB) geometry provides the means for elucidating the role of HB on stability of molecular structures.

At ambient conditions, in FOX-7 crystal, space group P2₁/n, each molecule is linked with six adjacent molecules through the extensive network of intermolecular N–H···O hydrogen bonds [2]. This arrangement stabilizes the structure and leads to the formation of wave-shaped layers. As shown in Figure 1, there are total 12 intermolecular bonds; two of each kind. The N···O bond length varies from 2.89 Å (bond 3) to 3.16 Å (bond 2), and the N–H···O angle varies from 120° (bond 5) to 152° (bond 1). Accordingly, these hydrogen bonds can be classified as medium and weak strength bonds [20,21]. The difference in bond lengths and angles results in the anisotropic hydrogen bonding network; with the stronger bonds between molecules within the ribbons than molecules in the adjacent ribbons, see Figure 1.

Upon deuteration, it is expected that the hydrogen bonds in FOX-7 will become weaker due to the shortening of covalent N–H and lengthening of the intermolecular H···O bonds. Here we utilize

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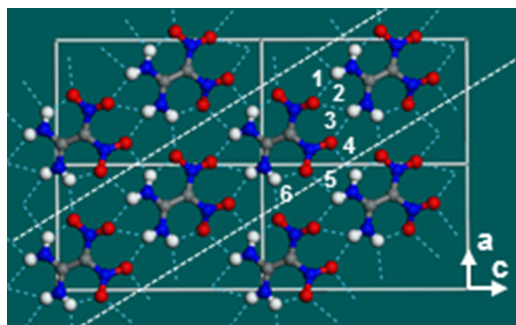


Figure 1. Projection of a FOX-7 layer on the (101) plane. The white-dashed lines mark 'the ribbons' of the head-to-tail arrangement of molecules in the layer. Molecules are represented by the ball-and-stick model. Hydrogen bonds are denoted by blue-dashed lines. Numbers denote six different types of hydrogen bonds. Legend: carbon, gray; nitrogen, blue; oxygen, red; hydrogen, white. Crystal unit cells are represented by white solid lines.

the above and mass effects by examining changes in the vibrational spectra using high-pressure Raman spectroscopy. We compare the FOX-7-d₄ results with those reported previously for FOX-7 to gain insight into the role of hydrogen bonding on the high-pressure stability of FOX-7. In particular, by altering the hydrogen bonding, we examine the contribution of hydrogen bonding to high-pressure effects in FOX-7: chemical stability, polymorphic transformations, and vibrational modes coupling.

2. Experimental procedures

A fine powder of FOX-7 was received from Dr. Joel R. Carney of Naval Surface Warfare Center-Indian Head Division (NSWC-IHD). FOX-7-d₄ was prepared according the procedure conveyed to us by Drs. David T. Boruta and Alfred G. Stern from NSWC-IHD. The method used in this work based on a general method reported for the NH group and described in Ref. [22]. To induce a proton exchange, 0.1 g of FOX-7 was dissolved in 5% NaOD. A solid product (FOX-7-d₄) was precipitated out by adding D₂SO₄, then washed by D₂O, and finally collected by filtration. The deuterium incorporation in FOX-7 was determined using ¹H NMR measurements. The chemical shifts of FOX-7 and FOX-d₄ as solutions in DMSO-d₆ were measured against respective residual solvent peaks. Integration of chemical shift peaks for N-H (δ = 8.80 ppm) gave the overall D-incorporation in FOX-7 better than 95%. The distribution of residual H atoms in deuterated FOX-7 molecules was not further examined. Single crystals of FOX-7-d₄ were grown by recrystallization of FOX-7-d₄ from acetone-d₆ solution at room temperature. These crystals had a rectangular shape, and were cut to dimensions required for high-pressure experiments. Typical dimensions of the crystals used in this study were $\sim(30 \times 30 \times 20) \mu\text{m}^3$.

High pressure was generated using a modified Merrill-Bassett type diamond-anvil-cell (DAC). A rhenium gasket, pre-indented to 0.05 mm with a 0.12 mm hole drilled in the indentation, was used as the sample compartment. Cryogenically loaded nitrogen was used as a pressure transmitting medium and pressure was determined from the frequency shift of R-lines of ruby crystal [23]. The precision of our pressure measurements was estimated to be 0.05 GPa.

The 532 nm line from a continuum wave diode-pumped solid-state laser was employed for Raman excitation. A micro-Raman system (T64000, JY-Horiba) equipped with a microscope was used; it provided a spectral resolution of $\sim 0.8 \text{ cm}^{-1}$. Experimental details regarding our micro-Raman and ruby fluorescence measurement techniques can be found elsewhere [24–26]. The positions and intensities of Raman peaks at each pressure were determined by

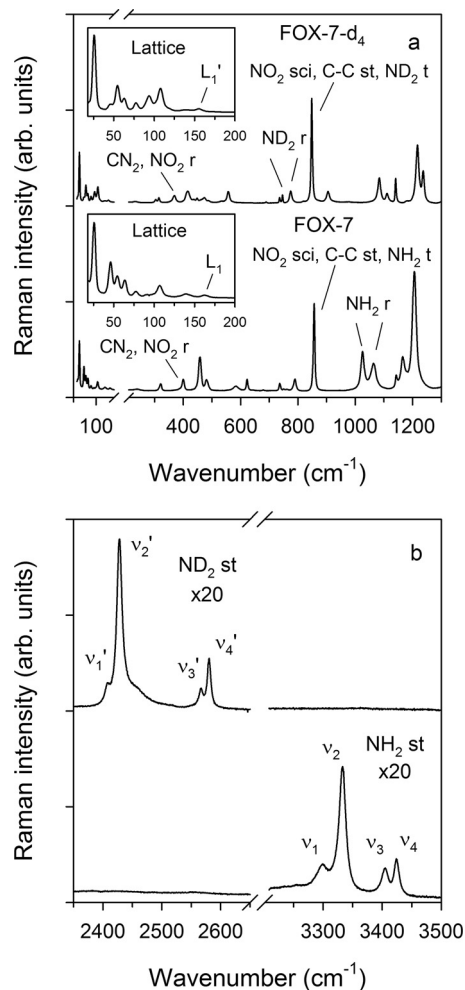


Figure 2. Raman spectra of FOX-7-d₄ and FOX-7 single crystals at ambient pressure in different frequency ranges: (a) from 0 to 1300 cm^{-1} and (b) from 2350 to 3500 cm^{-1} . The assignment of selected vibrations is provided [15]. The abbreviations used for the vibrations are the following: L: lattice, sci: scissoring, st: stretching, t: twisting, and r: rocking. Intensities of the spectra in the range 0–200 cm^{-1} were divided by 2.5. Insets show close-up views of spectra in the region of lattice modes. Intensities of spectra in panel 'b' are multiplied by 20 with respect to intensities of spectra in panel 'a'. Four NH₂ stretching vibrations and corresponding ND₂ vibrations are numbered from 1 to 4.

fitting the spectra to a Voigt (Gaussian–Lorentzian) function using a nonlinear least squares algorithm included in the PeakFit software.

3. Results and discussion

3.1. Ambient pressure

In Figure 2, we compare the Raman spectra of FOX-7-d₄ and FOX-7 at ambient pressure. The two spectra show differences in intensities and frequencies of various peaks. The former arise from the different orientations of FOX-7-d₄ and FOX-7 crystals with respect to the excitation beam. The latter, however, represents the actual effect of deuteration on the vibrational structure. As seen, the Raman peaks for the two spectra have very similar positions in the low frequency range. This occurs because the modes in this region are not associated with hydrogen, but contain the lattice and NO₂ twisting vibrations [15]. These are generally not affected by the substitution [27]. In contrast, the Raman peaks in the high frequency range show considerable shift to lower frequencies upon deuteration. The amount of shifts appears to depend on the extent of the NH₂ vibration contribution to the Raman peak. Accordingly,

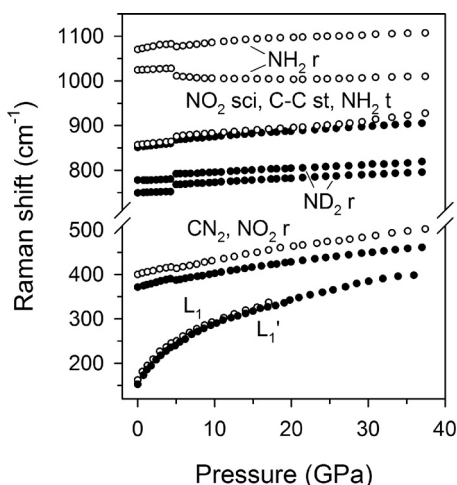


Figure 3. Pressure-induced shifts of selected Raman peaks of FOX-7-d₄ (solid circles) and FOX-7 (open circles). The assignment of FOX-7 modes is taken from Ref. [15]. The abbreviations used for the vibrations are the following: L: lattice, sci: scissoring, st: stretching, t: twisting, and r: rocking.

modes with little or no NH₂ vibration contributions, e.g., two mixed modes: (NO₂ scissoring, C–C stretching, NH₂ twisting) and (CN₂, NO₂ rocking) show very small shift. This can be seen for the very intense peak located at 856 cm^{−1}, composed of NO₂ scissoring, C–C stretching, and NH₂ twisting vibrations. This mode shifts only by few wavenumbers to 849 cm^{−1} upon deuteration, which is consistent with a small content of NH₂ vibrations. On the other hand, modes with pure NH₂ vibrations show significant red shifts. As seen in Figure 2, both stretching and rocking vibrations show these shifts. In the first case, four NH₂ stretching modes, two symmetric and two asymmetric, located at 3299, 3333, 3405, and 3425 cm^{−1} shift to 2407, 2428, 2566, and 2580 cm^{−1}, respectively in FOX-7-d₄. The calculated isotopic ratios (ISRs), $\nu(\text{NH}_2)/\nu(\text{ND}_2)$, for these modes are 1.37, for two symmetric and 1.33, for two asymmetric vibrations. These values are consistent with the 1.39 value expected from the ratios of reduced masses for these atoms. Similarly, two NH₂ rocking modes located at 1024 and 1070 cm^{−1} in FOX-7 show significant shift to 747 and 775 cm^{−1} respectively, in FOX-7-d₄, giving the ISR values of 1.37 and 1.38.

3.2. High pressure

In Figure 3, we compare pressure effects on the Raman shifts of selected vibrations upon deuteration. The results for other vibrations, in particular the NH₂ stretching modes, are presented in Section 3.2.2 to discuss changes in hydrogen bonding. It is evident that the pressure slopes for modes with small or no contribution of NH₂ vibrations are hardly affected by deuteration (Figure 3). On the other hand, the pressure shifts of ND₂ and NH₂ rocking vibrations are very different. In general, the ND₂ rocking modes shift at a smaller rate than the corresponding NH₂ modes. Also, the two ND₂ rocking modes show an increase in frequency at 4.5 GPa, in contrast to the decrease observed for the NH₂ modes. Finally, there is a clear reversal in the shift direction of one NH₂ rocking vibration at 4.5 GPa (1024 cm^{−1}), while the corresponding ND₂ rocking vibration (747 cm^{−1}) show no such change. The observed differences in pressure shifts of these modes are consistent with the shorter N–D bond as compared to the N–H bond.

3.2.1. Polymorphism and chemical stability

Our previous work on FOX-7 demonstrated discontinuities in the Raman shifts at 2 and 4.5 GPa, and full reversibility of the Raman spectra upon release from 40 GPa [9,10]. These results were

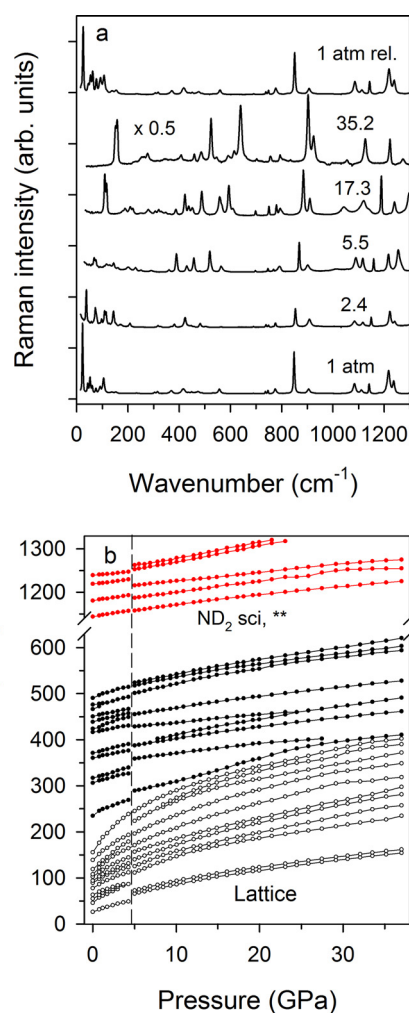


Figure 4. Pressure effects on the Raman spectra of FOX-7-d₄. (A) Selected spectra at several pressures in the frequency range from 0 to 1300 cm^{−1}. Pressure values are given in GPa next to each spectrum. The intensity of the spectrum at 35.2 GPa was divided by 2. The top spectrum was measured at ambient pressure after release from a pressure of 40 GPa. (B) Pressure-induced shifts of Raman peaks of FOX-7-d₄ in the frequency range from 0 to 1300 cm^{−1}. Results are represented by solid (internal modes) and open (lattice modes) circles. Red symbols represent modes containing mostly the ND₂ scissoring vibrations. ** Symbol denotes contribution from other types of vibrations. Lines are used to guide the eye. The vertical dashed line denotes discontinuity in the Raman peaks shift at 4.5 GPa. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

explained in terms of two phase transitions and retention of chemical stability at high pressures [10]. Here we examine how the H/D substitution affects these structural changes. To assess this, we show selected results of pressure effects on Raman spectra and Raman shifts of FOX-7-d₄ in Figure 4. As before, the experiments in this work were performed to 40 GPa. Typical results shown in Figure 4, panel 'a', reveal that the Raman spectra are fully reversible upon compression and subsequent release of pressure to ambient conditions. This behavior is similar to that observed for FOX-7, implying that the changes introduced to the molecular structure by deuteration are not sufficient to compromise the chemical stability.

Further analysis of the spectra reveals distinct discontinuities in pressure shifts of almost all Raman peaks at 4.5 GPa; exactly at the same pressure as for FOX-7 (Figure 4, panel 'b'). However, there are no changes in shifts around 2 GPa. These differing effects of deuteration on the behavior of FOX-7-d₄ at 2 and 4.5 GPa suggest a different role of hydrogen bonding on the transitions at these pressures. No change in the pressure onset for the transition observed at 4.5 GPa

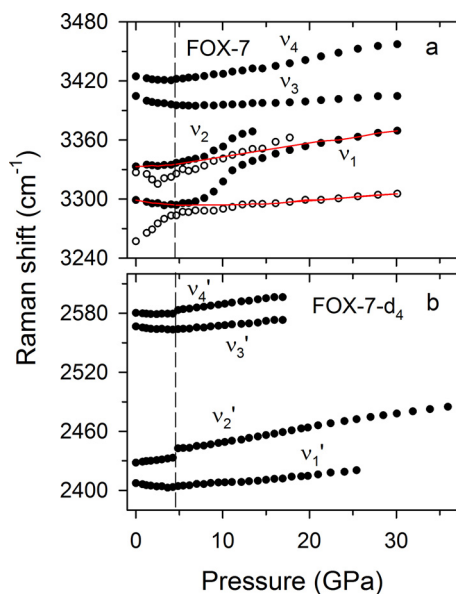


Figure 5. Pressure dependence of Raman shifts of NH_2 stretching (a) and ND_2 stretching (b) vibrations. Open circles denote peaks assigned to the combination modes [10]. Red solid lines represent the approximate expected shifts of ν_1 and ν_2 modes without perturbation by coupling. The vertical dashed line is drawn at 4.5 GPa. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

in FOX-7 indicates that either the modifications in hydrogen bonds upon deuteration are insufficient to alter this transition or this transition does not involve hydrogen bondings. The latter option can be ruled out, because we observed significant changes at the transition in modes related to NH_2 and ND_2 vibrations, see e.g., Figures 3 and 4 (panel 'b'). Therefore, it appears that forces leading to phase change at 4.5 GPa dominate the perturbations introduced by deuteration.

On the other hand, an absence of discontinuities at 2 GPa implies that deuteration eliminates spectral changes at this pressure, and likely removes this transition. The FOX-7 results showed that changes in Raman shifts at 2 GPa: (i) involve only few peaks, (ii) include small discontinuities or changes in slope, and (iii) involve mostly modes with NH_2 vibrations contribution. These features were tentatively attributed to a subtle phase transition, involving molecular conformational changes. The absence of these features in FOX-7- d_4 suggests further that this transition can be associated with hydrogen bonds.

3.2.2. D-bonding vs H-bonding: ND_2 and NH_2 stretching vibrations

The behavior of hydrogen or deuteron bonding under high pressure can be monitored through changes in the NH_2 or ND_2 stretching vibrations. In FOX-7, there are four NH_2 stretching vibrations: two symmetric, 3299 and 3333 cm^{-1} , and two asymmetric, 3405 and 3425 cm^{-1} . In FOX-7- d_4 these modes assume frequencies 2407, 2428, 2566, and 2580 cm^{-1} respectively. The pressure effects on these modes are compared side by side for FOX-7 and FOX-7- d_4 in Figure 5. In FOX-7, two symmetric vibrations couple with two combination modes under high pressure [10]. Thus, only approximate shifts for the uncoupled vibrations could be obtained (red lines in Figure 5, panel 'a'). However, deuteration removes this coupling, providing the pressure dependence for the unperturbed vibrations. From this, we find that anomalies in the shifts of ν_1 and ν_2 modes at the lower end of pressure are not due to the coupling but due to the phase transition. Also, the results in Figure 5 panel 'b', confirm that the pressure onset of transition at 4.5 GPa is not affected by deuteration.

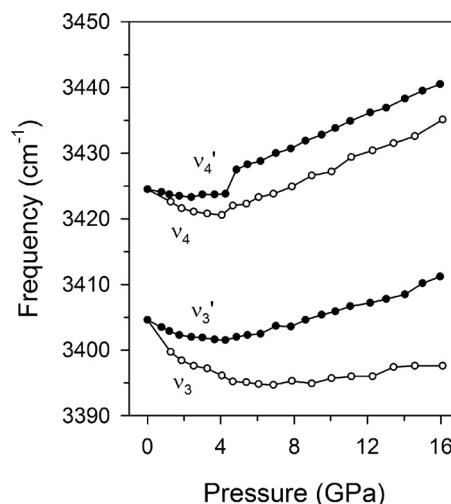


Figure 6. Pressure dependence of Raman shifts of asymmetric NH_2 (ν_3 and ν_4) and ND_2 (ν_3' and ν_4') stretching vibrations. The frequencies of ND_2 modes were shifted by the same amount so that they matched values of NH_2 modes at ambient pressure. Lines are drawn to guide the eye.

Detailed differences in pressure shifts of ND_2 and NH_2 stretching vibrations are presented in Figure 6. The asymmetric vibrations were selected for comparison, since they are not perturbed by coupling. To facilitate the comparison, the frequencies of ND_2 modes, ν_3' and ν_4' , were shifted by the same amount so that they matched values of NH_2 modes, ν_3 and ν_4 , at ambient pressure. As can be seen, the two modes for FOX-7 and FOX-7- d_4 exhibit red shift with initial compression. This result implies lengthening of the covalent N–H and N–D bonds, and thus, the strengthening of the intermolecular $\text{H} \cdots \text{O}$ and $\text{D} \cdots \text{O}$ bonds. However, the ND_2 vibrations show smaller rate of shift than the corresponding NH_2 vibrations. This behavior is consistent with the initial stronger attraction in the $\text{H} \cdots \text{O}$ bonding than in the $\text{D} \cdots \text{O}$ bonding [28,29]. However, as previously stated, this difference does not shift or eliminate the transition at 4.5 GPa.

One can also see in Figure 6, that the red shift reverses to blue shift around 4.5 GPa. This likely results from the fact that the H- and D-bonds experience repulsions from the surrounding neighbors in the crystal confinement, which prevent further expansion of the covalent N–H and N–D bonds. Furthermore, similar rates of shifts of corresponding modes for FOX-7- d_4 and FOX-7 above 4.5 GPa imply that the H/D substitution plays a lesser role in affecting the stability of the high-pressure phase.

3.2.3. Vibrations coupling

In FOX-7, we observed several instances of intensity exchange between various modes and avoided crossing of frequencies with increasing pressure, indicating the modes coupling [10]. The modes coupling was quantitatively analyzed in terms of Fermi resonance model and normal modes analyses [10,15]. The most widespread coupling was observed in the 600–900 cm^{-1} range and in the region of NH_2 stretching vibrations. The respective regions are shown in Figures 7 and 5, panels 'a', as we compare the results of FOX-7 with those of FOX-7- d_4 . Of particular interest are couplings in the 600–900 cm^{-1} range, since they involve the C– NO_2 vibrations. We suggested that the coupling of these modes with NH_2 or other vibrations may have implication for the shock insensitivity of FOX-7 [10]. We argued that energy imparted to the crystal from the shock cannot be easily localized in C–N motions, thus the higher energy (stress) would be required to break the bond.

The results of this work demonstrate that the couplings between various modes are removed by deuteration. We have shown this above for the NH_2 stretching vibrations, and here we show

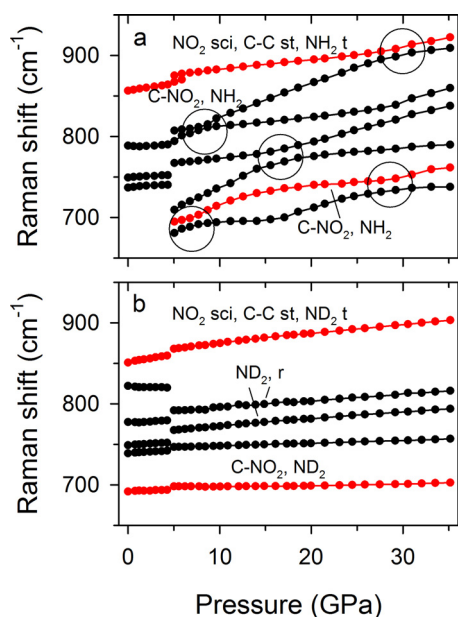


Figure 7. Pressure dependence of Raman shifts of selected modes, illustrating the changes in modes coupling upon deuteration. Experimental points are connected with lines to guide the eye. Red symbols are used to mark the corresponding modes of FOX-7 and FOX-7-d₄. (A) FOX-7; circles indicate the pressure regions of resonance coupling between different modes [10]. (B) FOX-7-d₄.

for modes in the range 600–900 cm⁻¹. The latter is presented in Figure 7, where the numerous couplings between different vibrations in FOX-7 are indicated by the circles. However, the examination of Figure 7, panel 'b', reveals the absence of modes coupling in the same frequency range in FOX-7-d₄, e.g., the modes presented in red color do not have their coupling counterparts. Also, there was no apparent evidence for the modes coupling in the remaining frequency ranges. The removal of modes coupling is likely a combined product of the increase in the reduced masses of hydrogen related bonds and of the decrease in the strength of hydrogen bonding. If the modes coupling contribute to the decreased shock sensitivity of FOX-7, then one should expect that FOX-7-d₄ to be more sensitive to shock initiation. This hypothesis merits examination in shock experiments.

4. Conclusions

We used Raman spectroscopy and H/D substitution to achieve a better understanding of the role of hydrogen bonding on different aspects of the high-pressure stability of FOX-7 crystal. By weakening the hydrogen bonds through deuteration, we found that the two phase transitions, observed in FOX-7 at 2 and 4.5 GPa, were affected differently in FOX-7-d₄. The transition at 2 GPa is not observed in FOX-7-d₄, but the transition at 4.5 GPa occurs exactly at the same pressure as in FOX-7. Despite the different response to deuteration,

we suggest that both transitions are due to changes in hydrogen bonding. Furthermore, this work demonstrates that the deuteration does not compromise the high-pressure chemical stability of FOX-7 under static compression. The FOX-7-d₄ crystal was unchanged by compression to 40 GPa and a subsequent release of pressure, as assessed from a full reversibility of the Raman spectra. Finally, we found that deuteration lifts the vibrational modes coupling, which occurs to a great extent in FOX-7. Because of the proposed association of modes coupling with shock insensitivity of FOX-7, this result may indicate increased shock sensitivity for FOX-7-d₄. Shock experiments are required to examine this conjecture.

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