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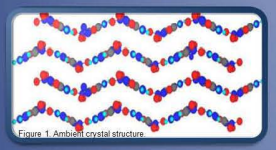


Figure 1. Ambient crystal structure.

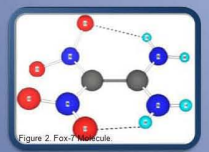
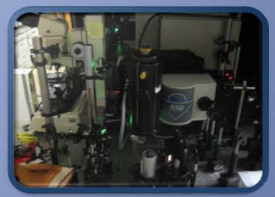
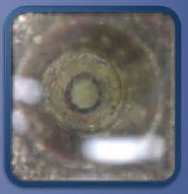


Figure 2. Fox-7 Molecule.





Abstract

The goal of this experiment is to better understand the reasons for Fox-7's insensitivity and high performance. It is very similar to other explosives in composition but different in structure. This different structure is believed to be the reason for Fox-7's unique characteristics. Using Raman spectroscopy along with high pressure techniques we hope to better understand this molecule and how it handles extreme conditions.

Introduction

1,1-diamino-2,2-dinitroethene (Fox-7) is an insensitive secondary explosive that was developed recently by Sweden. Thus there is very little known about it. The material is known to form a zig zag crystalline pattern as seen in Figure 1. The molecule itself consists of two carbon atoms connected by a double bond, one carbon has two amino groups and the other has two nitro groups. The structure of the molecule is shown in Figure 2. The molecule is also known to have hydrogen bonding[1].

This explosive, or energetic material, has a higher insensitivity and performance than RDX, making it a more ideal explosive. A higher insensitivity means that it takes a higher energy to start a reaction and thus it is less likely to be detonated unintentionally, while it maintains the desired performance when detonated[1].

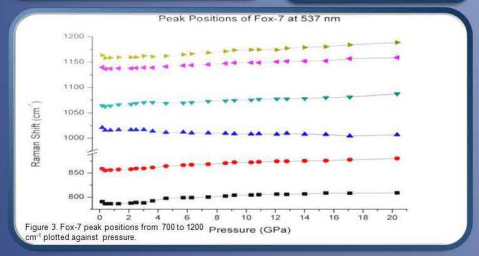


Figure 3. Fox-7 peak positions from 700 to 1200 cm^{-1} plotted against pressure.

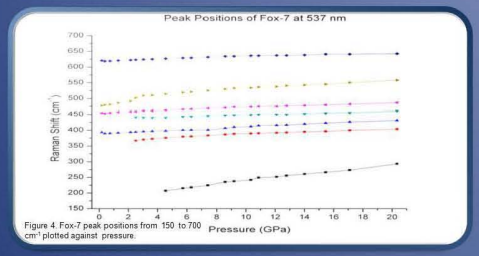


Figure 4. Fox-7 peak positions from 150 to 700 cm^{-1} plotted against pressure.

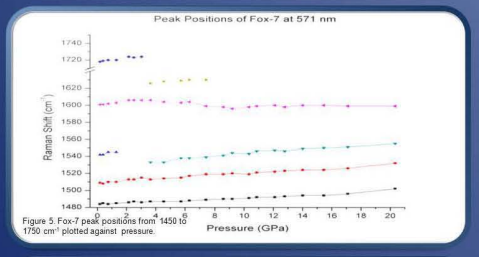


Figure 5. Fox-7 peak positions from 1450 to 1750 cm^{-1} plotted against pressure.

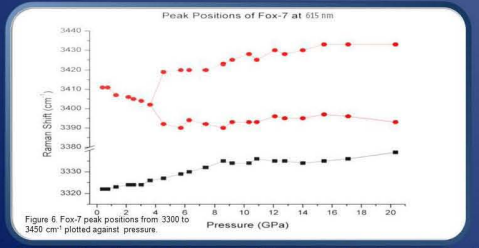


Figure 6. Fox-7 peak positions from 3300 to 3450 cm^{-1} plotted against pressure.

Procedure

A diamond anvil cell (DAC) was loaded with Fox-7 and no medium in a stainless steel gasket. The DAC used was a Merril-Basset design and had a pair of 400 micron diamonds. The gasket was preindented to about 60 microns in thickness and then a 145 micron hole was drilled for the sample. The sample was loaded with ruby sphere, which would be used to measure pressure. Once the DAC was loaded and a spectrum of the ruby was taken to find the initial pressure. The Raman spectrum was then collected on the Fox-7 at 537, 571 and 615 nm, 0-1400, 1400-2500 and 2700-3700 cm^{-1} Raman Shifts respectively. The pressure was then increased and the ruby and sample were scanned again and this process continued until a pressure of 20.34 GPa was reached with approximately 1 GPa steps. The DAC was then decompressed to ambient pressure and a spectrum was taken of the sample again. A spectrum of a new sample of Fox-7 was then taken to measure the ambient spectrum of the sample prior to compression. The data was then analyzed and the peaks were mapped against pressure and the spectrums were stacked according to pressure.

Conclusion

Figures 4, 5 and 6 show strong evidence of a phase transition around 3 GPa by the appearance and disappearance of peaks. Upon further inspection Figures 3 and 7 also support this with a change in the shift of peaks. Figures 3, 4 and 8 show evidence of a phase transition around 5 GPa with the strongest evidence being the appearance of a peak in Figure 4. Figures 6 and 7 show evidence of another phase transitions around 9-10 GPA. The change in the shift of the lowest peak in Figure 6 is the strongest evidence of this. The phase transitions are believe to be in largely due to a change in hydrogen bonding and possibly a change from the zig zag crystal pattern to a planar crystal pattern.

To further study these phenomena an analysis of each peak should be done to determine what vibrational mode it corresponds to. From there you could see which vibrational modes are involved in each phase change to help understand what is happening on the molecular level during the transitions.

References

1. Lochert J., Ian. Fox-7- A New Insensitive Explosive. DSTO-TR-1238
2. Galley, Martin. Raman Studies of 1,3,5,7 Cyclooctatetraene at High Pressure

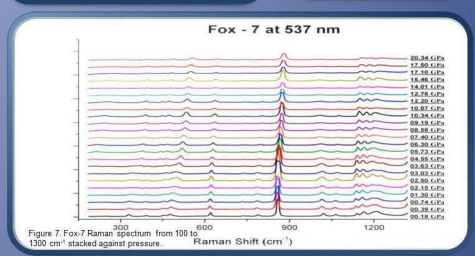


Figure 7. Fox-7 Raman spectrum from 100 to 1300 cm^{-1} stacked against pressure.

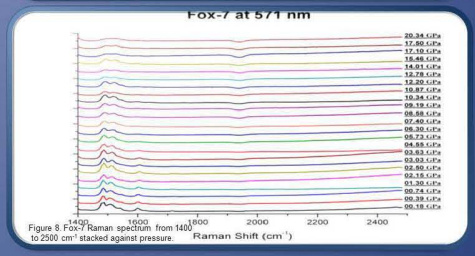


Figure 8. Fox-7 Raman spectrum from 1400 to 2500 cm^{-1} stacked against pressure.

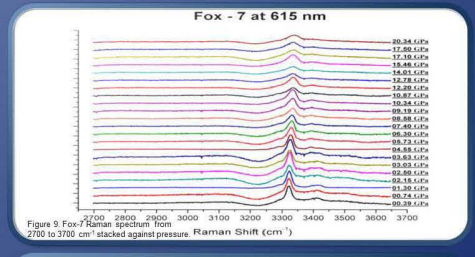


Figure 9. Fox-7 Raman spectrum from 2700 to 3700 cm^{-1} stacked against pressure.

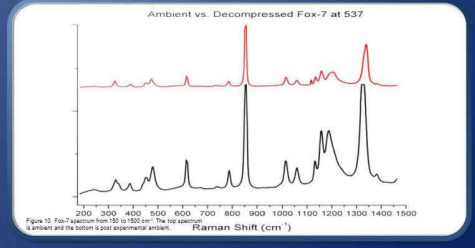


Figure 10. Fox-7 spectrum from 150 to 1500 cm^{-1}. The top spectrum is ambient and the bottom is post experimental ambient.

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