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# Identification of a Cyclopentyl Nitrite Inhalant

**ABSTRACT:** A submission of an acidic yellow liquid was found to consist of cyclopentyl nitrite, an alkyl nitrite compound that has not appeared in forensic literature. As no commercial standards were available, a comparison standard was synthesized. Thirteen commercial alkyl nitrite products were purchased and examined and each was found to contain butyl nitrite, regardless of commercial content labeling.

**KEYWORDS:** Cyclopentyl Nitrite, Cyclopentyl Nitrate, Cyclopentanol, Butyl Nitrite, Poppers

Amyl and Butyl Nitrite inhalants, produced by reacting sodium nitrite with amyl or butyl alcohol, are vasodilators that are inhaled to enhance sexual pleasure. Nitrite inhalants also cause vasodilatation, with brief hypotension, dizziness, and flushing, followed by reflex tachycardia (1). These products, known as "Poppers", are typically sold in specialty shops as over-the-counter products labeled as head cleaners or air fresheners.

An unmarked brown glass vial was seized in a traffic stop of an erratic driver. The vial contained a clear, yellow tinted acidic (pH 1-2) liquid that had a strong solvent odor.

A vapor phase infrared spectrum (Figure 1) revealed the liquid to consist of a non-aromatic nitrite compound, but inconsistent with the commonly encountered amyl and butyl nitrite and the uncommon but previously reported cyclohexyl nitrite[i]. Capillary gas chromatography-mass spectrometry of the liquid indicated a cyclopentanol moiety.

## Materials and Methods

Vapor phase infrared spectra were collected by placing a drop of liquid in a gas cell (International Crystal Laboratories 8-054 equipped with KBr windows) and examined via a Fourier transform infrared spectrometer (Perkin Elmer Spectrum One with mid-range MCT detector).

Gas chromatography-mass spectrometry data were obtained by drawing a 10 ul sample of the container headspace in a gas-tight Hamilton syringe and injecting into a Thermo-Finnigan Trace Gas Chromatograph-Mass Spectrometer (EI), equipped with a 15M x 0.25mm ID DB-5 column with a 0.25mm film thickness. The initial oven

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temperature was 40° C, held for 5 minutes and ramped to 200° C at a rate of 25° C per minute.

Ion chromatography was performed by diluting the samples in analytical grade water (NERL Diagnostics 9800-1) and the anions separated on a Dionex DX-120 Ion Chromatograph, equipped with an AS9-HC (Dionex 4 x 250mm) column. A laboratory prepared 9mM sodium carbonate eluent mobile phase was used with a flow rate of 1.2 ml/min. under isocratic conditions.

## Results

Gas Chromatography-Mass Spectrometry of the questioned liquid headspace showed the presence of three major peaks at 1.18, 1.37 and 2.37 minutes (Figure 1).

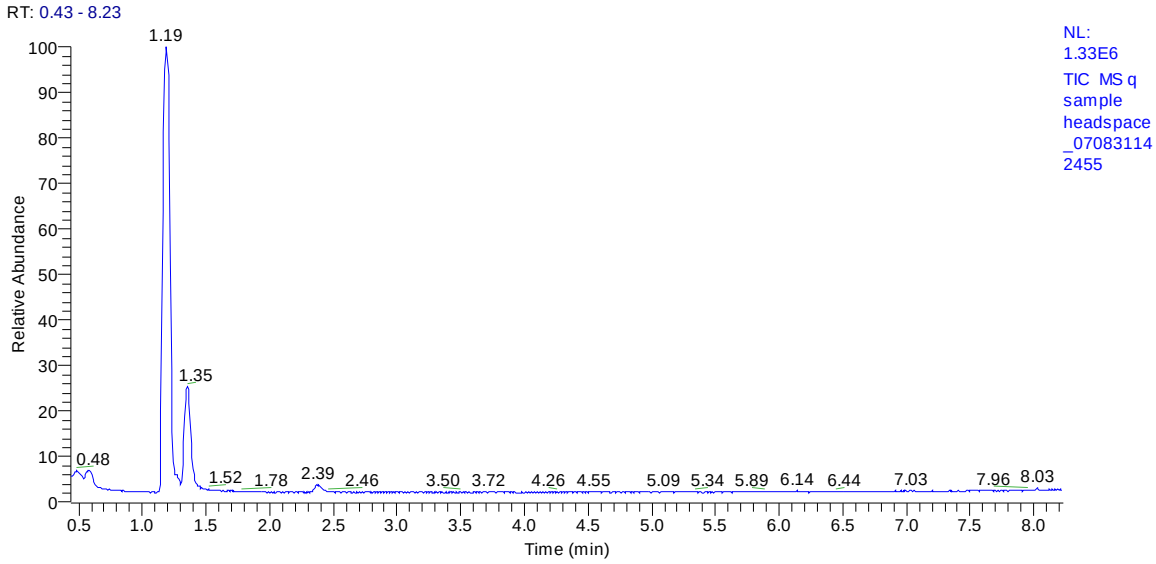


FIG 1- *Gas chromatogram of questioned liquid headspace*

The compound eluting at 1.19 minutes had a 41 base peak and major ions at 55, 57, 67, 69 and 84 (Figure 2). A search of the instrument's NIST library identified the compound as "Cyclopentanol, nitrate, Formula $C_5H_9NO_3$, CAS #21823-29-0". An internet search for this compound and CAS number did not reveal any information.

The compound eluting at 1.37 minutes had a 57 base peak with major ions at 44, 67 and a molecular ion of 86. This component was identified using a reference standard as cyclopentanol (Figure 3).

The compound eluting at 2.37 minutes also displayed a 57 base peak and major ions at 44, 67 and a molecular ion of 86. This compound was identified using the NIST reference library as 2-pentanol, distinguished from cyclopentanol based on ion ratios.

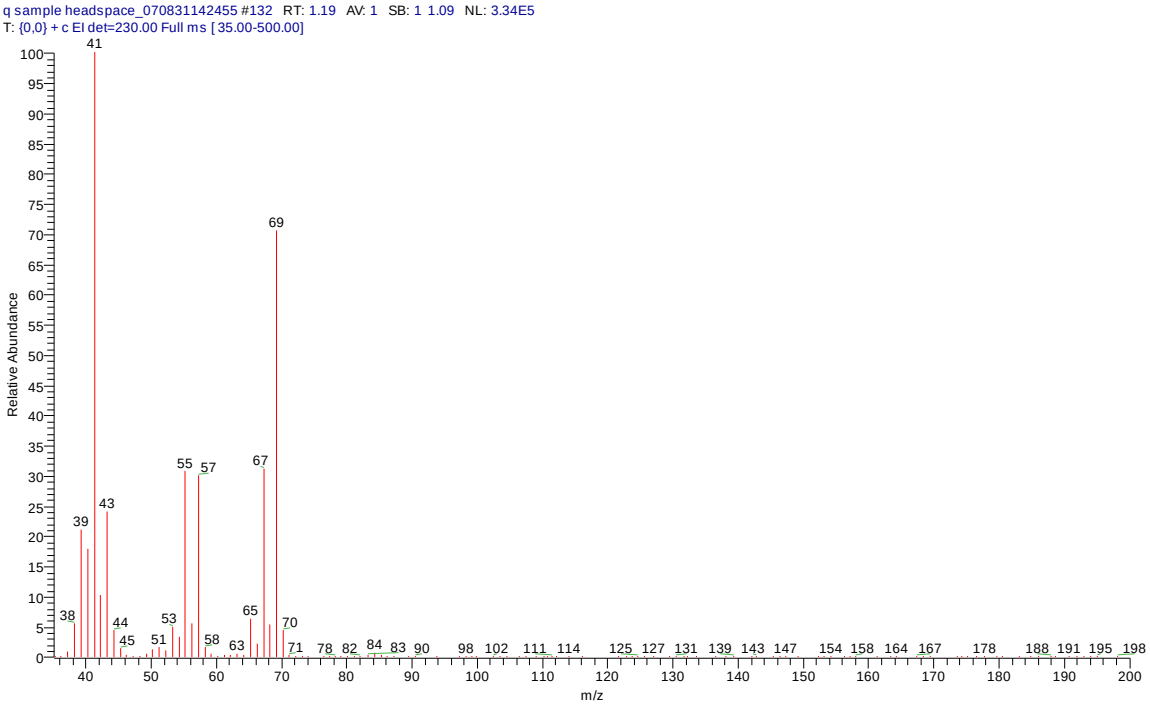


FIG. 2- *Mass spectrum of the case sample's peak eluting at 1.19 min. This peak is consistent with cyclopentyl nitrite.*

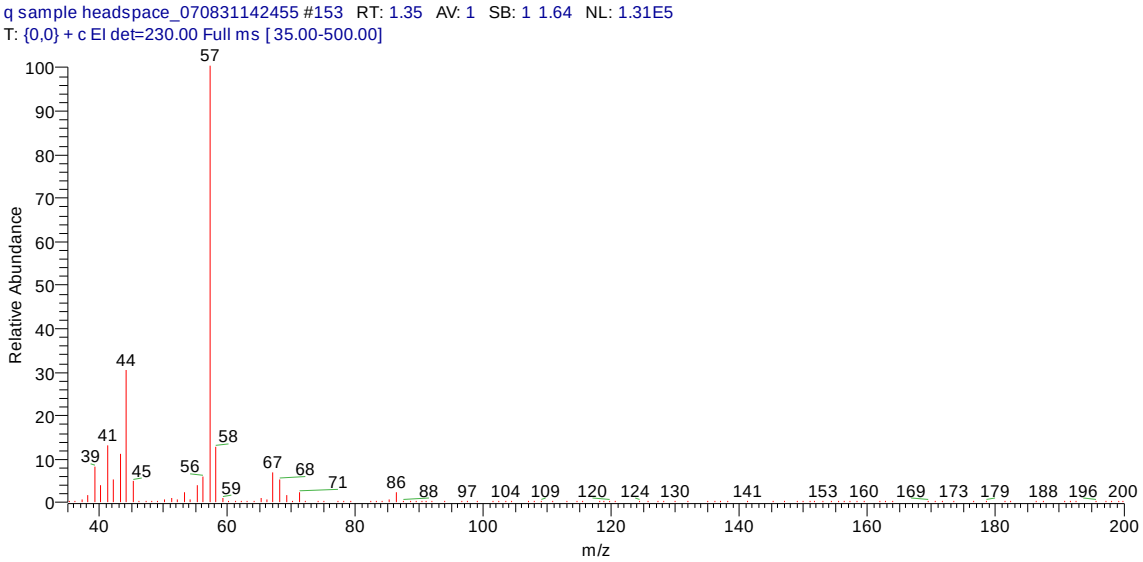


FIG. 3- *Mass spectrum of the case sample's peak eluting at 1.35 min. This peak is consistent with cyclopentanol.*

It was suspected by the author that the compound identified by the NIST library as "Cyclopentanol, nitrate" was actually cyclopentyl nitrite. The structure of cyclopentyl nitrate appears unstable and it was surmised that the compound would be reduced in solution to the nitrite of the compound (Figure 4). Neither cyclopentyl nitrate nor

cyclopentyl nitrite had been reported in the forensic literature nor do either have a commercially available analytical standard.

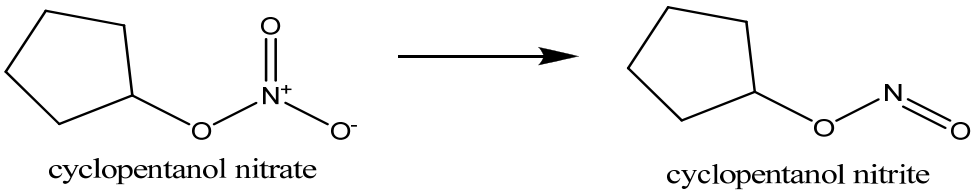


FIG. 4- *Reduction of Cyclopentyl Nitrate to Cyclopentyl Nitrite*

An attempt to manufacture a cyclopentyl nitrite standard was made by reacting cyclopentanol (99%, Alfa Aesar, Heysham, England) with potassium nitrite (ACS, Fisher Scientific, Fair Lawn, NJ) in con. sulfuric acid (ACS, Fisher Scientific, Fair Lawn, NJ) No visible reaction occurred and FTIR and GC-MS examination of the product indicated no detectable cyclopentyl nitrite was produced. The cyclopentanol was then reacted with ammonium nitrate (ACS, Mallinckrodt, St. Louis, MO) in con. sulfuric acid. This resulted in a sustained exothermic reaction resulting in a yellow liquid with a pH of 1-2, similar to the questioned liquid in the case. Vapor phase IR spectra and headspace GC-MS data were obtained under the same conditions as the questioned liquid and confirmed the compounds produced in the reaction were consistent with the known liquid (Figures 5, 6, 7).

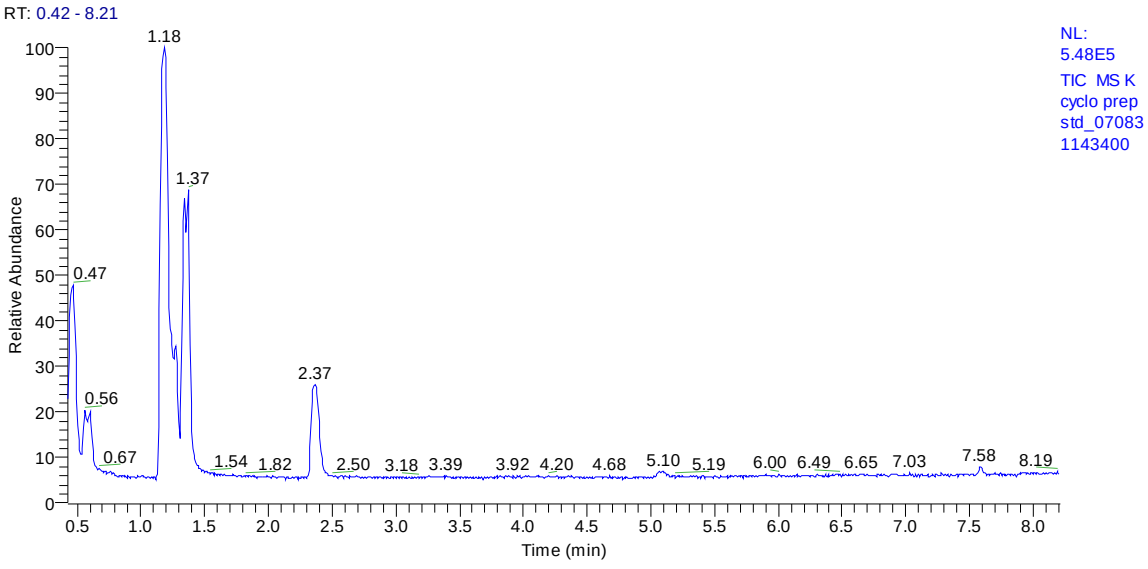


FIG. 5- *Gas chromatogram of headspace of liquid produced from cyclopentanol, ammonium nitrate and sulfuric acid.*

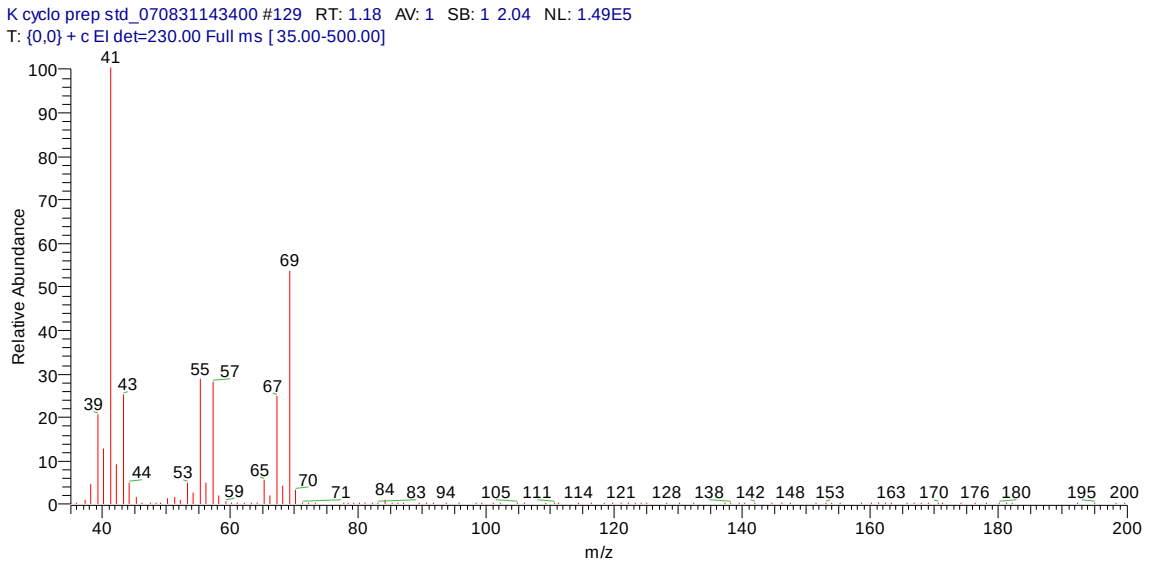


FIG. 6–*Mass spectrum of the laboratory prepared sample peak eluting at 1.18 min. This peak is consistent with cyclopentyl nitrite.*[2]

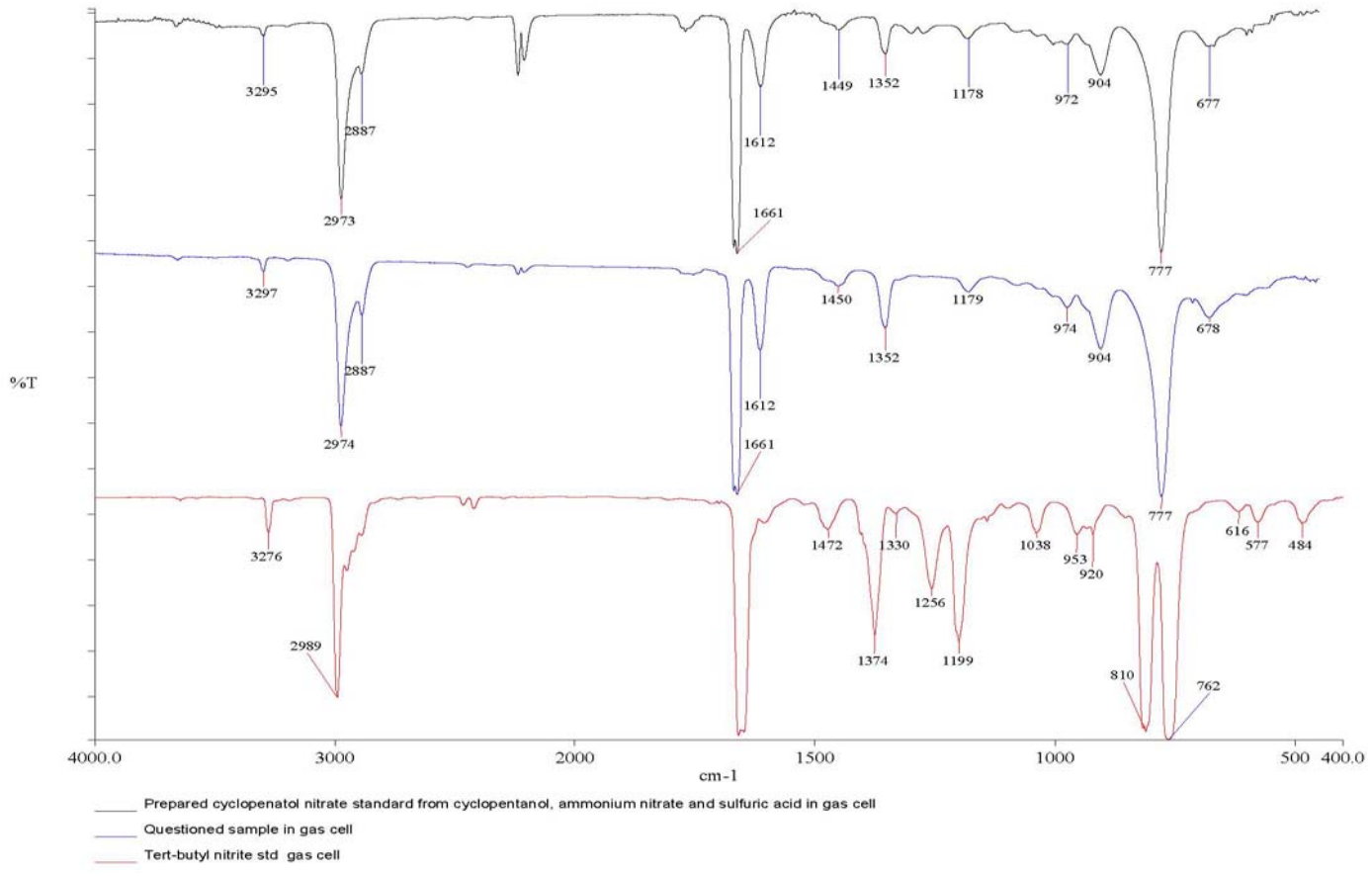


FIG. 7–*Vapor phase infrared spectrum of prepared cyclopentyl nitrite standard (top/black), questioned sample (middle/blue) and butyl nitrite (bottom/red).*[2]

[2] *Figure titles corrected following errata published in JASTEE 6-3.*

To determine if the reaction product was cyclopentyl nitrite or cyclopentyl nitrate, ion chromatography was performed. The retention times of the reacted liquid were compared to that of a standard anion mixture (Dionex #56933) and found to consist primarily of nitrite with a trace amount of nitrate present. This finding was sufficient along with the FTIR and GC-MS analytical data to confirm both the standard synthesized from cyclopentanol, ammonium nitrate and sulfuric acid and the questioned sample as containing cyclopentyl nitrite. Three commercial alkyl nitrite products (Blue Boy, Jungle Juice and Crypt Tonight) were also examined by this method and also found to show the presence of nitrite anions.

In an attempt to locate a commercial product containing cyclopentyl nitrite, thirteen commercial "Popper" samples were purchased and analyzed via gas phase FTIR and GC-MS in the same manner as described above. The results are listed in Table 1.

| Product Name | Label Content | Compounds Detected |
|---|---|---|
| Jungle Juice Plus Room Odorizer | Isopentyl Nitrite | Butyl Nitrite, Butyl Alcohol |
| Crypt Tonight Head Cleaner | 85% isobutyl alcohol, 5%HCl, 5% H2O, 5% Other | Butyl Nitrite, Butyl Alcohol |
| PowR PeleT Video Head Cleaner | 85% isobutyl alcohol, 5%HCl, 5% H2O, 5% Other | Butyl Nitrite, Butyl Alcohol |
| Mr. Chaps Leather Cleaner | 85% isobutyl alcohol, 5%HCl, 5% H2O, 5% Other | Butyl Nitrite, Butyl Alcohol |
| Amsterdam Poppers | Alkyl Nitrate | Butyl Nitrite, Butyl Alcohol |
| Can Opener Cleaner | Anaerobic Stabilizer Resin | Butyl Nitrite, Butyl Alcohol |
| Jim Diamond's 24k Cleaner | Anaerobic Stabilizer Resin | Butyl Nitrite, Butyl Alcohol |
| Zap! Cleaner | Anaerobic Stabilizer Resin | Butyl Nitrite, Butyl Alcohol |
| Purple Video Head Cleaner | Cyclohexyl Nitrite | Butyl Nitrite, Butyl Alcohol |
| Nitro Supra Liquid Aroma | Does not contain Alkyl Nitrites | Butyl Nitrite, Butyl Alcohol |
| Blue Boy Liquid Incense | Isobutyl Nitrite | Butyl Nitrite, Butyl Alcohol |
| Pig Sweat Polish Remover | None | Butyl Nitrite, Butyl Alcohol |
| Ecstasy Pop | None | Butyl Nitrite, Butyl Alcohol |

TABLE 1- *Results of commercial alkyl nitrite analysis. All products contained butyl nitrate, regardless of label content.*

All the commercial products examined were found to contain butyl nitrite and butyl alcohol. This was regardless of the commercial labeling which indicated that the products contained various ingredients, including isopentyl nitrite, cyclohexyl nitrite and other substances. One labeled product, "Nitro Supra" indicated that the product "does not contain alkyl nitrites", yet upon examination, butyl nitrite was also found in this product. None of the products examined showed the presence of cyclopentyl nitrite.

## Discussion

It appears that while butyl nitrite is the most commonly sold over-the-counter nitrite inhalant, manufacturers/distributors of many of these products may use a number of alkyl nitrate compounds and not appropriately label the packaging. It was not determined whether cyclopentyl nitrite inhalant that was encountered in this case was clandestinely produced or used as an ingredient of a commercial nitrite inhalant. If it was a commercial product, it may have not been labeled as containing this material.

## References

(1) Dearmore, I., Cyclohexyl Nitrite Encounter, J Forensic Sci 1999; 44(1):197-204

(2) Porter, RS, et al., The Merck Manual Online, Merck & Co., Retrieved on 8-12-08., http://www.merck.com/mmpe/sec15/ch198/ch198m.html#sec15-ch198-ch198m-400