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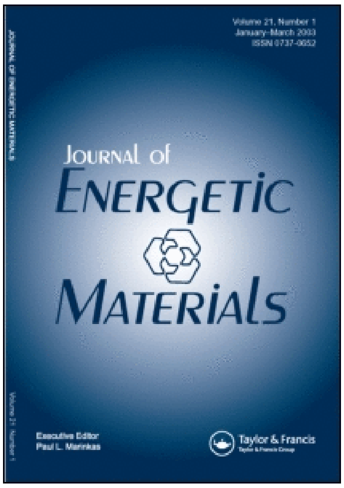

Journal of Energetic Materials
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713770432

N''-nitro-N-(2,2,2-trinitroethyl) guanidine

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To cite this Article Christe, Karl O. , Frankel, Milton B. and Weber, James F.(1987) 'N''-nitro-N-(2,2,2-trinitroethyl) guanidine', Journal of Energetic Materials, 5: 1, 83 — 85
To link to this Article: DOI: 10.1080/07370658708012351
URL: http://dx.doi.org/10.1080/07370658708012351

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RESEARCH NOTE

N"-NITRO-N-(2,2,2-TRINITROETHYL) GUANIDINE

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ABSTRACT

The previously reported compound N-nitro-N'-(2,2,2-trinitroethyl) guanidine (3) is shown by ^{1}H NMR spectroscopy to be actually the corresponding nitrimine tautomer N"-nitro-N-(2,2,2-trinitroethyl) guanidine (4).

Nitramines are of interest as explosives because of their high and rapid energy release.[1] For this application a high nitrogen and oxygen content is desirable. This goal can be achieved by the introduction of, for example, a trinitroalkyl group into a molecule such as nitroguanidine.

In a previous report,[2] the reaction of nitroguanidine (1) with formalin was stated to produce methylolnitroguanidine (2) which when reacted with trinitromethane produces N-nitro-N'-(2,2,2-trinitroethyl) guanidine (3).

$$\underset{1}{\mathrm{NO_2NHC(NH)NH_2}} \xrightarrow{+\mathrm{CH_2O}} \underset{2}{\mathrm{NO_2NHC(NH)NHCH_2OH}} \xrightarrow{+\mathrm{CH(NO_2)_3}}$$

$$\underset{3}{\mathrm{NO_2NHC(NH)NHCH_2C(NO_2)_3}}$$

Journal of Energetic Materials vol. 5, 83-85 (1987)

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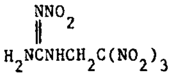
Unpublished work in our and several other laboratories has confirmed the formation of a product having the composition and physical properties reported for 3. However, some of the chemical properties of this product cast doubt on the correctness of the previously assigned[1] structure. To clarify the structure of this compound its proton NMR spectrum was recorded at 25°C in perdeuterated dimethyl sulfoxide solution using TMS as an internal standard. The compound exhibited three signals at δ8.35, 7.80 and 5.20 with an area ratio of 2:1:2. The δ8.35 and 7.80 signals were a broad singlet and triplet, respectively, and the δ5.20 signal consisted of a sharp doublet. Based on the observed line widths, chemical shifts and area ratios, these signals are attributed to an $-NH_2$, $=NH$, and $=CH_2$ group, respectively. The observed coupling between the $=CH_2$ and the $=NH$ group was 7Hz with the broadening of the $-NH_2$ and $=NH$ lines being due to the quadrupole moment of the ^{14}N nucleus.

The above spectrum leaves no doubt that the previously reported structure 3 is incorrect and that the product of the above reaction is the tautomeric nitrimine 4.



$H_2N\overset{NNO_2}{\overset{\|}{C}}NHCH_2C(NO_2)_3$

4

After completion of our study we have learned about the results of a recent crystal structure determination which confirms structure 4 for the above material.[3] This finding is also in agreement with a previous report[4] that nitroguanidine itself exists primarily in the nitramine form $(H_2N)_2C=NNO_2$.

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ACKNOWLEDGEMENT

We thank the Air Force Rocket Propulsion Laboratory, Air Force Systems Command, USAF, Edwards AFB, California, for financial support of this work.

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