CONTINUED COMPUTATIONAL EVALUATION OF THE FEASIBILITY OF NITRATING PRECURSORS TO C$_{12}$N$_{12}$O$_{12}$.

by

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Continued Computational Evaluation of the Feasibility of Nitrating Precursors to $C_{12}N_{12}O_{12}$

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Extending the work reported in Technical Report No. 71 (October 20, 1994), we computed the average local ionization energies on the surfaces of two more possible precursors to 1. No minima were found at the positions to be nitrated, indicating that these are not favored sites for this purpose.

$C_{12}N_{12}O_{12}$, nitration, average local ionization energies

Unclassified

Unclassified

Unclassified

Unlimited

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Introduction

In Technical Report No. 71 (October 20, 1994), we investigated the susceptibility to electrophilic attack involving charge transfer (as in nitration) of several possible precursors to 1. We computed the average local ionization energies $\bar{I}_S(r)$ on the surfaces of 2 - 4 (Figure 1) in order to determine the ease of charge transfer at positions a and b. At the request of M. L. Trudell, we have now extended this study to include 5 and 6. The procedure used was the same as described in the earlier report, which also discusses the definition and interpretation of $\bar{I}_S(r)$. The results are given in Figure 1, together with those obtained previously.

![Chemical Structures](image1)

We find no minimum in $\bar{I}_S(r)$ at positions a in 5 and 6, which is consistent with what was observed earlier for 4. This indicates that these are not favorable sites for charge transfer to an electrophile.

![Chemical Structures](image2)
Figure 1. Some Computed (STO-5G) Minima of Average Local Ionization Energies on Molecular Surfaces

- NO$_2$
  - a = 15.4 eV
  - b = 15.1 eV
  - c = 15.2 eV

- NO$_2$
  - a = 16.4 eV
  - b = 16.2 eV
  - c = 15.8 eV

- O$_2$N
  - a = 17.2 eV

4. a: no minimum;
   $\bar{I}_S(r) = \text{approx. } 15.9 \text{ eV.}$
   b = 15.2 eV

2. a = 16.3 eV

3. a = 16.6 eV

5. a: no minimum;
   $\bar{I}_S(r) = \text{approx. } 16.8 \text{ eV.}$

6. a: no minimum;
   $\bar{I}_S(r) = \text{approx. } 17.0 \text{ eV.}$