Crystal Structure of 1,4,5,8-Tetranitronaphthalene, Form II

By JAMES R. HOLDEN and CHARLES DICKINSON*

(*U.S. Naval Ordnance Laboratory, White Oak, Silver Spring, Maryland* 20910)

THE geometry of polynitroaromatic compounds has been the subject of extensive studies.[1,2] Dashevskii *et al.*[3] proposed a method, based on a model suggested by Kitaigorodskii,[4] for determining the geometry of such molecules. To investigate the accuracy and applicability of this method we determined the structure of 1,4,5,8-tetranitronaphthalene by conventional *X*-ray methods.

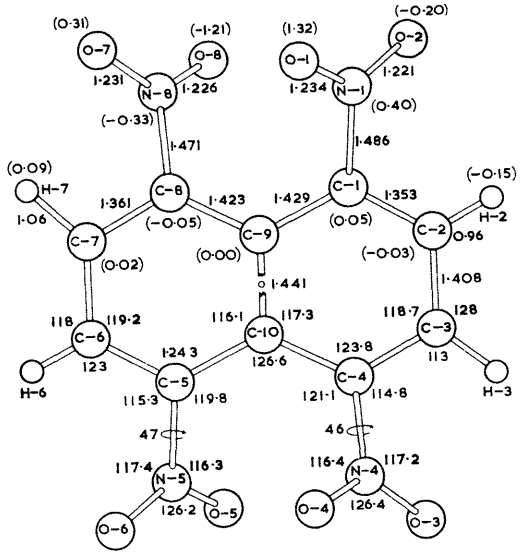

FIGURE. *Bond lengths and angles of* 1,4,5,8-*tetranitronaphthalene, form II.*

Some confusion exists as to the physical properties of 1,4,5,8-tetranitronaphthalene, especially of its melting point; according to our results its m.p. is >400°.[5] Further, it has two polymorphic forms with a solid–solid transition at *ca.* 260°. The room-temperature stable polymorph (form II) crystallizes in space group $P2_1/c$, with $a = 5{\cdot}38$, $b = 7{\cdot}71$, $c = 13{\cdot}55$Å, $\beta = 92{\cdot}7°$, D_m 1·80, $Z = 2$, $D_c = 1{\cdot}82$ g. cm.$^{-2}$.[6]

The intensity data was collected using an integrating Weissenberg camera and processed on a semi-automatic densitometer. The structure was solved by Patterson and full-matrix least-squares techniques to a conventional R of 0·10 using anisotropic temperature factors. The structure at this point consists of 111 parameters and is based on 801 observed data.

The bond lengths and angles are given in the Figure, with the numbers in parentheses representing deviations (in Å) from the best plane through the carbon skeleton. The average errors in bond lengths are $\pm 0{\cdot}007$Å and in bond angles are $\pm 0{\cdot}5°$ for the non-hydrogen atoms. To relieve the severe crowding caused by the *peri*-substituents, the nitro-groups are rotated (46° and 47°), wagged (13° and 16°), and splayed. The interior angles are consistent with the hypothesis of Carter *et al.*[7] concerning the effect of electron-withdrawing groups on bond geometry. There are no indications of significant intermolecular interactions.

We thank Dr. H. G. Adolph of these laboratories for providing the sample and the Foundational Research Fund of the U.S. Naval Ordnance Laboratory for financial support.

(*Received, December 6th,* 1968; *Com.* 1669.)

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