THE CRYSTAL STRUCTURE OF
p-AZO-TOLUENE (CH₃-C₆H₄N)₂

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Kapadia¹ has studied the unit cell dimensions of p-azo-toluene. Its crystal
structure has not been reported in literature so far. The present paper gives
the complete structure by X-ray diffraction studies.

UNIT CELL AND SPACE-GROUP

p-azo-toluene crystallizes in the form of thin narrow flat plates, the longer
dimension being parallel to the b-axis. Rotation and Weissenberg photo-
graphs taken with the three crystallographic axes as axis of rotation gave the
following cell data.

\[ a = 12.01 \text{ Å}; \quad b = 5.02 \text{ Å}; \quad c = 9.32 \text{ Å} \quad \text{and} \quad \beta = 90° 12'. \]

The number of molecules per unit cell is 2. From the systematic absent
reflections the space-group was confirmed to be \( \text{C}_{2h}^\infty - P 2_1/a \).

INTENSITY MEASUREMENTS AND STRUCTURE DATA

The structure amplitudes were obtained from Weissenberg photographs
(Cu-Kₐ radiation) using multiple film technique. The normal beam method
was adopted for all photographs. The intensities were estimated visually
by comparison with standard intensity spots. They were corrected for
Lorentz, polarisation and temperature factors and later put on the absolute
scale by the statistical method of Wilson. No absorption correction was
made as the crystals used were very small.

DETERMINATION OF THE STRUCTURE

Since there are only two molecules per unit cell, each molecule must
have a centre of symmetry. A Patterson projection using \((h 0 l)\) reflections
was made, but it failed to give any clear indication of the benzene ring.
Hence the method of ‘trial and error’ was adopted. As a first attempt
the N–N bond of the two planar benzene rings was assumed to lie in the
same plane as the rings. Because the molecule has a centre of symmetry
such an assumption leads to the conclusion that the two rings must be
coplanar. Structure factors were calculated with this structure. It was
noticed that no amount of adjustment could bring an agreement between the observed and the calculated structure factor values.

![Diagram of p-azo-toluene structure](image)

**Fig. 1.** Final electron density projection of p-azo-toluene on (ac) plane. Contours at arbitrary intervals.

A second series of trials was made with the two benzene rings attached by a central zig-zag bond, as in the case of dibenzyl. This gave structure