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CRYSTALLOGRAPHIC DATA OF MESOGENIC
4, 4'-BIS (HEPTYLOXY) AZOXYBENZENE

The mesogenic compound 4, 4'-bis (heptyloxy) azoxy
benzene with the structural formula

\[
\text{H}_2\text{C}=\text{O} - \text{N} - \text{N} - \text{O} - \text{C}_7\text{H}_{15}
\]

4-4'-bis (heptyloxy) azoxybenzene

exhibits, on heating, the following liquid crystalline
phases:

Solid \(73^\circ C\) smectic (C) \(95^\circ C\) nematic \(123^\circ C\) isotropic.

This has been confirmed from our observation on the
phase transition of this substance using a hot stage
in conjunction with a polarizing microscope as well
as from X-ray Laue Photograph studies. The refractive
indices and densities at different temperatures have
been determined and already reported\(^1\). Presently we
have carried out preliminary X-ray investigations on
these crystals.

Large rectangular plaque type yellow crystals were
grown from benzene solution. Rotation and Weissenberg
photographs along different axes were recorded
using optically homogeneous crystals (as verified by
observing the crystals under a polarising microscope).
From these photographs the unit cell dimensions and
space group were determined using the standard

---

The relevant crystal data thus obtained are:

Molecular formula: \(\text{C}_{46}\text{H}_{84}\text{N}_{2}\text{O}_{5}\), Molecular weight: 426.6, Space group: \(\text{P}1\) or \(\text{P}1\), \(a = 8.61 \pm 0.04 \text{Å}\), \(b = 10.82 \pm 0.04 \text{Å}\), \(c = 14.70 \pm 0.04 \text{Å}\), \(a = 98^\circ 48'\), \(\beta = 102^\circ 18'\), \(\gamma = 95^\circ 31'\), \(z = 2\), \(\rho_{\text{exp}} = 1.13 \text{ g/cc}\), \(\rho_{\text{cal}} = 1.08 \text{ g/cc}\).

The crystal belongs to space group \(\text{P}1\) or \(\text{P}1\), which is explainable\(^2\) on the basis of imbricated packing as there are two molecules per unit cell.

The authors are thankful to Prof. D. Krishnamurti
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ESTIMATION OF URANIUM IN PLANT
AND WATER SAMPLES

Estimation of traces of uranium in plant and water
samples is carried out by using fission track technique.
The uranium content in plants varies from 0.26 ppm
to 15 ppm with its maximum concentration in hydro-
phytes. Water samples show a variation in uranium
content from 1 ppb to 19 ppb.

Introduction

It is well known that trace quantities of uranium
are present in almost all substances. Fission track
 technique provides an ingenious method for trace
estimation of uranium in plant and water samples.
The technique first developed by Price and Walker\(^1\)
was applied with success by Fleischer and Lovett\(^2\)
for uranium estimation in water and by Nagpal \textit{et al.}\(^3\)
for uranium estimation in plants.

Our present investigations are based on the study
of eight plant samples collected from the different
ecological habitats in the Punjab University campus
and three water samples collected from the Matiarkan
and Deng hot water springs and from the University
water supply.
Experimental Procedure

Uranium estimation in plant samples is made by using a technique developed by Fisher and known as homogenized fission track analysis. This technique is most suitable for samples having heterogeneous distribution of uranium and it proves quite efficient even in the ppb range provided thermal neutron dose is properly specified.

Plant samples are dried in an oven till the material is completely charred. This residue is powdered and pulverized. 50 mgm of the plant residue is thoroughly mixed with 100 mgm of methyl cellulose which acts as a binder and the mixture is pressed into a pellet of 1-3 cm dia. and 1 mm thickness by a hand pressing machine. Similar pellets are prepared from different species of plants.

Lexan plastic discs of the same diameter as that of pellets are cut out and pressed against both sides of each pellet. The lexan discs are used as external detectors for recording fission tracks. The pellets are then packed in an aluminium capsule which is irradiated with a specified thermal neutron dose of 10^12 (nvt) in the thermal column of Cirrus Reactor at B.A.R.C., Trombay.

After irradiation the lexan discs are removed from the pellets and etched in 6 N NaOH solution at 70°C for 20 minutes using a reflux condenser. The replicate discs are scanned under Carl Zeiss binocular microscope using a magnification of 600 X and etched induced fission tracks are counted over the whole surface. The tracks are also counted on a blank lexan sample irradiated along with the pellets to find error due to laboratory contamination.

Uranium concentration is determined by comparing mean track densities recorded in lexan discs covering plant pellets with those covering the standard glass dosimeter pellet (which is packed and irradiated in the same capsule with the same dose) by using the formula:

\[
\frac{C_w (\text{sample})}{C_w (\text{standard})} = \frac{\rho (\text{sample})}{\rho (\text{standard})}
\]

(1)

where \(C_w\) represents the uranium concentration and \(\rho\) the induced track density.

Experimental procedure for preparation of water samples is different from the case of plant samples. A known volume of water (2 drops = 0.04 c.c.) of each sample is taken on lexan plastic discs and allowed to evaporate. The non-volatile constituents of water are left over the discs in the form of a thin film. The irradiation and etching procedure adopted is the same as described in the case of plant samples. The induced fission tracks were counted over the entire surface of the 3 pairs of detector discs for each sample of water and the uranium concentration determined by using the formula:

\[
C_w = \frac{TM}{VG N_A \sigma E \phi}
\]

(2)

where

- \(N_A\) = Avogadro number (6.023 × 10^23),
- \(\sigma\) = fission reaction cross-section (4.2 × 10^{-24} cm^2),
- \(M\) = atomic weight of uranium isotope (238),
- \(V\) = volume of water (0.04 c.c.),
- \(\phi\) = total thermal neutron dose (10^12 nvt),
- \(T\) = total number of tracks counted over detector disc,
- \(G\) = geometry factor which is taken as unity, and
- \(E\) = etching efficiency factor, \([E = 1 - (V_U/V)\])^2 approx. equal to 1 for lexan plastic.

Discussion of Results

Uranium contents of plant and water samples calculated by using eqns. (1) and (2) are summarized in Tables I and II, respectively. From the experimental

<table>
<thead>
<tr>
<th>Ecological group</th>
<th>Botanical name</th>
<th>Track Density ((\rho \times 10^9))</th>
<th>Uranium conc. (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Upper face</td>
<td>Lower face</td>
</tr>
<tr>
<td>Hydrophytes</td>
<td><em>Hydrilla</em> sp.</td>
<td>150.0</td>
<td>171.0</td>
</tr>
<tr>
<td></td>
<td><em>Salvia</em> sp.</td>
<td>260.0</td>
<td>286.0</td>
</tr>
<tr>
<td>Mesophytes</td>
<td><em>Dahlia</em> sp.</td>
<td>7.4</td>
<td>6.7</td>
</tr>
<tr>
<td></td>
<td><em>Lathyrus Oederatus</em></td>
<td>22.5</td>
<td>20.5</td>
</tr>
<tr>
<td></td>
<td><em>Lilium</em> sp.</td>
<td>25.0</td>
<td>35.0</td>
</tr>
<tr>
<td></td>
<td><em>Tropaeolum majus</em></td>
<td>10.5</td>
<td>15.0</td>
</tr>
<tr>
<td>Xerophytes</td>
<td><em>Russus</em> sp.</td>
<td>10.0</td>
<td>14.8</td>
</tr>
<tr>
<td></td>
<td><em>Bryophyllum</em> sp.</td>
<td>8.4</td>
<td>10.2</td>
</tr>
</tbody>
</table>
analysis, it is observed that uranium content in various plant species varies from 0·26 ppm to 15·0 ppm. Plant samples have been divided into three groups, viz., hydrophytes, mesophytes and xerophytes. There is maximum accumulation of uranium in hydrophytes which may be due to their capacity of fixing uranium from water. The uranium content in mesophytes and xerophytes is of the same order though much less than that in hydrophytes.

**Table II**

<table>
<thead>
<tr>
<th>Source of water</th>
<th>Total number of tracks (T)*</th>
<th>Uranium Conc. (ppb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laboratory tap water</td>
<td>$1.63 \times 10^6$</td>
<td>19·2</td>
</tr>
<tr>
<td>Manikaran hot springs</td>
<td>$1.23 \times 10^6$</td>
<td>15·0</td>
</tr>
<tr>
<td>Deng hot springs</td>
<td>$9.19 \times 10^4$</td>
<td>1·1</td>
</tr>
</tbody>
</table>

* Mean of 6 observations.

Nagpal et al. also find same relative order of uranium contents in the three ecological classes of plants, though the U values in the case of individual plants do not agree. The counting statistical errors in our results are less than 5%. However the track count variation in replicates of some plant samples goes up to 35% which is evidence of inhomogeneous distribution of uranium in plants.

The fission track analysis of water samples reveals maximum uranium content in laboratory tap water. This anomaly may be attributed to laboratory contamination such as radioactive dust due to storage of uranium samples and needs further investigation. Manikaran water contains 15 ppb uranium and Deng water contains only 1·1 ppb. The depletion of uranium in hot water springs is probably due to the increased chemical reactivity of hot waters and the removal of uranium minerals early in the life of hot springs.

**Conclusions**

1. Fission track technique can prove to be a valuable tool for botanical and hydrogeochemical prospecting of uranium.
2. It can also be used to detect radioactive pollution of our environment in the vicinity of U mining areas.

Authors are thankful to Dr. S. L. Koul for collection of water samples and to Sh. R. K. Bawa for technical assistance. One of the authors (H. K.) is grateful to UGC for the award of teacher fellowship during the tenure of which this work is undertaken.

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HARINDER KAUR.


**MORSE FRANCK-CONDON FACTORS AND r-CENTROIDS FOR SOME WERNER BANDS OF H₂ AND D₂**

Morse Franck-Condon factors for the Morse potential and $r$-centroids have been computed for 144 Werner bands of the astrophysically important $H_2$ and $D_2$ molecules using new rotational and vibrational constants. The value of $\Delta r \equiv r_{v'\sigma'} - r_{v\sigma}$ in a sequence is found to remain constant. The Franck-Condon factors derived for the Morse potential may be used in conjunction with experimentally determined band oscillator strengths for five Werner bands (C-X system) of $H_2$ to derive radiative lifetimes which are inconsistent with the experimental lifetime measurements.

The growing interest of astronomy in the region of vacuum ultra-violet has led many workers to study the spectra of $H_2$ and $D_2$ which are in abundance in the interstellar space. Since new rotational and vibrational constants are available for the $B\Sigma^+_u$ and $C^1\Pi_u$ states of $H_2$ and $D_2$, the study of Franck-Condon factors and related quantities are needed.

Neglecting the variation of electronic transition moment of the molecule with nuclear motion, the relative intensities of the bands of a system of diatomic molecule are largely governed by Franck-Condon factors given by the following expression (Herzberg$^1$):

$$q_{\nu'\nu} = \int \psi_{\nu'}^* \psi_{\nu} \, dr \quad ^2$$

where $\psi_{\nu'}$ and $\psi_{\nu}$ are vibrational wave-functions of the upper and lower vibrational levels having quantum numbers $\nu'$ and $\nu$ respectively. The analytical method of Fraser and Jarmain$^2$ with $r$-shift correction has been employed for the evaluation of Franck-Condon factors of the Werner bands of $H_2$ and $D_2$. The experimental molecular parameters for the $B\Sigma^+_u$, $C^1\Pi_u$ and $X\Sigma^+_g$ states as reported by Herzberg and Howe$^1$. 