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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
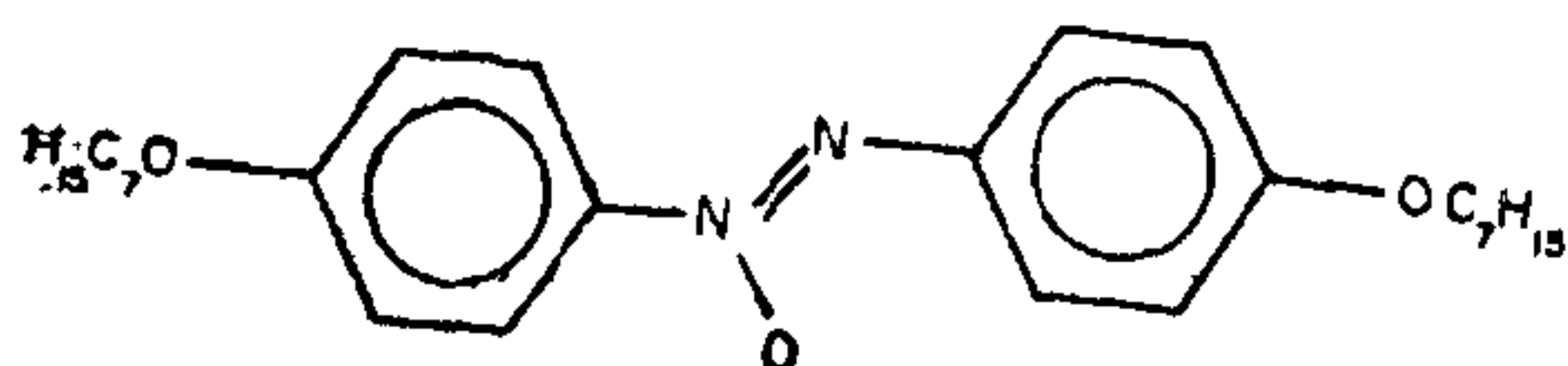
4-4'-bis (heptyloxy) azoxybenzene

exhibits, on heating, the following liquid crystalline phases :

Solid $\underline{73°C}$ smectic (C) $\underline{95°C}$ nematic $\underline{123°C}$ 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

techniques[2]. The relevant crystal data thus obtained are :

Molecular formula: $C_{26}H_{38}N_2O_3$, Molecular weight: 426·6, Space group : P1 or P$\bar{1}$, $a = 8·61 \pm 0·04$ Å, $b = 10·82 \pm 0·04$ Å, $c = 14·70 \pm 0·04$ Å, $a = 98° 48'$, $\beta = 102° 18'$, $\gamma = 95° 31'$, $z = 2$, $\rho_{exp.} = 1·13$ g/cc, $\rho_{cal.} = 1·08$ g/cc.

The crystal belongs to space group P1 or P$\bar{1}$, which is explainable[3] on the basis of imbricated packing as there are two molecules per unit cell.

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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 hydrophytes. 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[1-2] was applied with success by Fleischer and Lovett[3] for uranium estimation in water and by Nagpal *et al.*[4] 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 Punjabi University campus and three water samples collected from the Manikaran 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[3] and known as homogenised 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 aluminium capsule which is irradiated with a specified thermal neutron dose of 10^{17} (nvt) in the thermal column of Cirus 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 30 minutes using a reflux condenser. The replicate discs are scanned under Carl Zeiss binocular microscope using a magnification of 600 × 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[6]

$$\frac{C_{w} \text{ (sample)}}{C_{w} \text{ (standard)}} = \frac{\rho \text{ (sample)}}{\rho \text{ (standard)}} \tag{1}$$

where C_{w} represents the uranium concentration and ρ 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[3]

$$C_{w} = \frac{TM}{V \, G \, N_{A} \sigma E \, \phi} \tag{2}$$

where

N_{A} = Avogadro number ($6·023 \times 10^{23}$),
σ = fission reaction cross-section ($4·2 \times 10^{-24} \, cm^{2}$),
M = atomic weight of uranium isotope (238),
V = volume of water (0·04 c.c.),
ϕ = total thermal neutron dose (10^{17} nvt),
T = total number of tracks counted over detector disc,
G = geometry factor which is taken as unity, and
E = etching efficiency factor,
$[E = 1 - (V_{g}/V_{t})^{2}$ 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 I

Uranium content in various plants species

Ecological group	Botanical name	Track Density ($\rho \times 10^{4}$)			Uranium conc. (ppm)
		Upper face	Lower face	Mean	
Hydrophytes	*Hydrilla* sp.	150·0	171·0	160·5	8·70
	Salvinia sp.	260·0	286·0	273·0	14·93
Mesophytes	*Dahlia* sp.	7·4	6·7	7·1	0·26
	Lathyrus Oderatus	22·5	20·5	21·5	1·05
	Lilium sp.	25·0	35·0	30·0	1·50
	Tropaeolum majus	10·5	15·0	12·8	0·58
Xerophytes	*Ruscus* sp.	10·0	14·8	12·4	0·55
	Bryophyllum sp.	8·4	10·2	9·3	0·38

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

Uranium content in water

Source of water	Total number of tracks (T)*	Uranium Conc. (ppb)
Laboratory tap water	$1·63 \times 10^6$	19·2
Manikaran hot springs	$1·23 \times 10^6$	15·0
Deng hot springs	$9·19 \times 10^4$	1·1

* Mean of 6 observations.

Nagpal *et al.*[4] 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 upto 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 uraninite 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[7].

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.

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MORSE FRANCK-CONDON FACTORS AND r-CENTROIDS FOR SOME WERNER BANDS OF H_2 AND D_2

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 $\Delta r \equiv r_{v'+1, v''+1} - r_{v', v''}$ 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 $B^1\Sigma^+_u$ 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]):

$$q_{v'v''} = \left| \int \psi_{v'} \psi_{v''} \, dr \right|^2$$

where $\psi_{v'}$ and $\psi_{v''}$ are vibrational wave-functions of the upper and lower vibrational levels having quantum numbers v' and v'' respectively. The analytical method of Fraser and Jarmain[2] with r_v-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 $B^1\Sigma^+_u$, $C^1\Pi_u$ and $X^1\Sigma^+_g$ states as reported by Herzberg and Howe[3],