



Figure 1. General view of the molecule along the b-axis.

1. The angles around the palladium ion are close to the expected 90° and 180° but there are some distortions due to slight strain caused by chelation. The N_1 -Pd- O_1 and N_2 -Pd- O_4 angles (83.4° and 85.4°) are smaller than the N_1 -Pd- N_2 and O_1 -Pd- O_4 angles (98.6° and 92.4°). The O_1 -Pd- N_2 and O_4 -Pd- N_1 angles (173.9° and 175.3°) are smaller than expected. The Pd- N_1 and Pd- N_2 lengths are 2.01 \AA and 2.01 \AA and the Pd- O_1 and Pd- O_4 lengths are 1.98 \AA and 1.99 \AA respectively. These are normal and agree with published data.⁵ The water molecules are not coordinated to the metal ion but are involved in hydrogen bonding with the

carboxylic oxygen and imino-nitrogen atoms. It appears that the hydrogen bonding involving water molecules is the predominant packing force in the crystal structure. In the pyrrolidine ring A, the atoms C_1 and C_5 are found to be on the opposite side of the coordination plane; C_1 and C_5 being below and above the plane respectively. The carboxyl group $O_1C_2O_2$ and the C_4 atom are in the trans position with respect to the plane of the ring. In the pyrrolidine ring B, deviations from the expected geometry and large thermal parameters for atoms C_8 and C_{10} have been found. Such deviations have been reported earlier for C_9 atom, in the complex *bis* (DL-proline) manganese (II)-dibromide dihydrate⁶. Since in the present structure C_9 is attached to a bulky hydroxyl group, it is felt that the distortion is manifest in C_8 and C_{10} atoms. Further refinement by assuming disordered state for the two atoms is in progress. Full structure details will be published in due course.

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NEUTRON DIFFUSION THROUGH A BARE PRISMATIC SOLID

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ABSTRACT

The problem of diffusion of neutrons through a bare prismatic solid with a cross-section of isosceles right triangle has been solved by the use of integral transform.

INTRODUCTION

THE neutron distribution in a fissionable solid is governed by the diffusion and multiplication of neutrons and is determined by the geometrical form of the solid. Hence the critical size depends on the geometry. The values of critical size for

geometries such as parallelo-piped cylinder, sphere and prism with equilateral triangular cross-section are known¹. We consider the diffusion of neutrons through a bare prismatic solid with cross-section as an isosceles right triangle. The solution of this problem is obtained by the use of integral transform and critical size is determined.

THE REQUIRED INTEGRAL TRANSFORM

Ugile¹ has developed an integral transform suitable for the isosceles right triangular boundary as

$$T[f(x,y)] = \bar{f}(m,n) = \int_0^a dx \int_0^{x^*} f(x,y) \theta_{m,n}(x,y) dy, \quad (1)$$

where the Kernel function θ is given by

$$\theta_{m,n}(x,y) = \sin[(m+n)\pi x/a] \sin[n\pi y/a] - (-1)^m \sin[(m+n)\pi y/a] \sin[n\pi x/a]. \quad (2)$$

with m and n as integers. The transform has the inversion formula,

$$f(x,y) = \sum_m \sum_n [4/a^2] \bar{f}(m,n) \theta_{m,n}(x,y). \quad (3)$$

STATEMENT OF THE PROBLEM

Consider the diffusion of neutrons through a bare prismatic solid of fissionable material of height h and with a cross-section perpendicular to the height as an isosceles right triangle of side a . Let there be no neutron sources inside the volume of the solid and the sizes a and h include extrapolation length.

According to the simple reactor model based on one group as discussed by Wayland², the diffusion of neutrons is governed by

$$D \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right] N + \frac{[k_c - 1]v}{\lambda} N = \frac{\partial N}{\partial t} \quad (4)$$

where $N = N(x,y,z,t)$, the neutron density, D = the thermal diffusion coefficient for neutrons, v = the thermal neutron speed, λ = absorption mean free path and k_c = average neutrons produced per absorption.

Here the Cartesian coordinate system is used with the bottom isosceles right triangle as the xy plane, and z axis along the height, the origin being at the corner of the right angle and x, y axes along the two equal and perpendicular sides of the bottom plane.

Since sizes of the solid are inclusive of extrapolation length, the neutron density will be zero at the boundary surfaces. Hence the boundary conditions will be

$$N(0,y,z,t) = 0, \quad N(x,0,z,t) = 0, \quad N(x,y,z,t) \text{ at } (x+y) = a \text{ is zero}, \quad (5)$$

$$N(x,y,0,t) = 0, \quad N(x,y,h,t) = 0. \quad (6)$$

SOLUTION OF THE PROBLEM

Applying the transform of (1) to (4) and simplifying it with the process of integration by parts and use of conditions (5), we get

$$-D [m^2 + 2mn + 2n^2] \frac{\pi^2}{a^2} \bar{N}(m,n,z,t) - D [\partial^2 / \partial z^2] \bar{N}(m,n,z,t) + \frac{(k_c - 1)v}{\lambda} \bar{N}(m,n,z,t) = \frac{\partial \bar{N}(m,n,z,t)}{\partial t}, \quad (7)$$

with the boundary conditions (6) transformed to

$$\bar{N}(m,n,0,t) = 0, \quad \text{and} \quad \bar{N}(m,n,h,t) = 0. \quad (8)$$

Further we apply finite sine transform of Kernel $\sin s\pi z/h$ with respect to z variable so that the problem given by (7) and (8) reduces to

$$\frac{\partial \bar{N}^*(m,n,s,t)}{\partial t} = \left[-D(m^2 + 2mn + 2n^2) \frac{\pi^2}{a^2} - D \frac{s^2 \pi^2}{h^2} + \frac{(k_c - 1)v}{\lambda} \right] \bar{N}^*(m,n,s,t), \quad (9)$$

where the star over the function represents its finite sine transform. The solution of this equation is

$$\bar{N}^*(m,n,s,t) = A_{mn} e \left[-D(m^2 + 2mn + 2n^2) \frac{\pi^2}{a^2} - D \frac{s^2 \pi^2}{h^2} + \frac{(k_c - 1)v}{\lambda} \right] t. \quad (10)$$

Applying the inversion formula (3) and the Fourier inverse finite sine transform to this, we obtain

$$N(x,y,z,t) = \sum_m \sum_n \frac{2}{\pi} \sin \left(\frac{s\pi z}{h} \right) \frac{4}{a^2} \left[\frac{\sin(m+n)\pi x}{a} \frac{\sin n\pi y - (-1)^m \sin(m+n)\pi y}{a} \frac{\sin n\pi x}{a} \right] A_{mn} e \left[-D(m^2 + 2mn + 2n^2) \frac{\pi^2}{a^2} + \frac{s^2 \pi^2}{h^2} + \frac{(k_c - 1)v}{\lambda} \right] t. \quad (11)$$

The A_{mn} values are the transforms of the neutron concentration initially such that the double summation on the right side of (11) with $t = 0$ converges to the initial concentration. If the exponent is with negative sign, the exponential term is less than unity for $t > 0$ and it can be proved by comparison with the situation at $t = 0$ that the double series in (11) converges.

SOLUTION AND MINIMUM CRITICAL VOLUME

In the expression (11) all terms, except the exponential, are bounded and the convergence or divergence of the double series is decided by the exponential term. If

$$\frac{(k_c - 1)v}{\lambda} = D \left[\frac{5\pi^2}{a^2} + \frac{\pi^2}{h^2} \right] \quad (12)$$

the contribution due to $m = 1, m = 1, s = 1$ will be independent of time; but for higher values of m, n and s the contributions will converge to zero with

increasing time. Hence the condition for sustained chain reaction with critical size of the specimen is,

$$\left[\frac{5\pi^2}{a^2} + \frac{\pi^2}{h^2} \right] = B^2 \quad (13)$$

where B is the material buckling given by

$$B^2 = [(k_c - 1)v] / \lambda D \quad (14)$$

The condition (13) leads to the critical volume of the prism, with isosceles right triangular base, as

$$V_{\min} = 201.5 / B^3 \quad (15)$$

The corresponding V_{\min} values for different geometries are given in table 1.

CONCLUSION

The study of diffusion of neutron through a prismatic solid of isosceles right triangular cross-section leads to the important result that this structure is useful for storage of the fissionable material as the minimum critical size is the highest in this case. Further, as the symmetry of the structure decreases the minimum critical size increases.

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TABLE 1

Minimum critical volume for different geometrics

Geometry of the solid	Minimum critical volume (B^3)
Sphere	130
Circular cylinder	148
Cube	161
Prism with equilateral triangular cross-section	186
Prism with isosceles right triangular cross-section	201.5

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BINUCLEAR ORGANOSILICON IMINE COMPLEXES, WITH SULPHUR DONOR BENZOTHIAZOLINE

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ABSTRACT

The condensation of salicylaldehyde with *o*-aminobenzenethiol involves the undesirable side reaction resulting in the ring closure with the formation of heterocyclic compound (benzothiazoline). It, however, appears to be in equilibrium with Schiff base form in solution. On reacting trimethylsilyl oxy-metal/non-metal isopropoxides with the ligand in the presence of cyclohexane, the anil form appears to react with isopropoxides and the equilibrium is shifted towards the formation of Schiff base complexes of these metals/non-metals. The resulting new derivatives having M—O—M' bonds have been characterized by elemental analyses, molecular weight determinations, conductance measurements and I.R., U.V. and PMR spectral studies.

INTRODUCTION

METAL chelation is involved in many important biological processes¹ and generally, the chelating ligands are polyfunctional molecules. Recently, much interest has been shown in the synthesis of metal chelates of sulphur containing ligands and it is within this particular area that rather

significant advances have been made². Studies pertaining to M—O—M' bonded imine complexes particularly with sulphur donor ligands are rather scanty. It was, therefore, considered of interest to prepare such types of complexes and the synthesis of complexes of the type, $\text{Me}_3\text{Si}-\text{O}-\text{M}_1(\text{ONS})$, $\text{Me}_3\text{Si}-\text{O}-\text{M}_2(\text{OPr}')_n(\text{ONS})$ and $\text{Me}_3\text{Si}-\text{O}-\text{M}_3(\text{ONS})_2$ [where $\text{M}_1 = \text{B(III)}, \text{Al(III)}, \text{La(III)}$ and Sm(III) ; $\text{M}_2 =$