

Fig. 1. Total cross section for H bound to  $C_{12}H_{10}$ .

The amplitude vectors calculated from the computed set of force constants were used, together with the measured vibrational frequencies, to construct the weighted frequency spectrum using in the slow neutron calculations.

The scattering law was computed, in the harmonic approximation, by means of the GASKET code.<sup>2</sup> The FLANGE code<sup>3</sup> was used to interpolate the scattering law

and to produce the scattering kernel. The total scattering cross section, the single differential cross section, as well as other neutron parameters, were calculated and compared with experimental data with gratifying results. Figure 1 shows the calculated total cross section and the comparison with experimental values.<sup>4</sup>

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2. J. U. KOPPEL, J. R. TRIPLET, and Y. D. NALIBOFF, GA-7417, General Atomic (1957).
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4. B. ANTONINI and A. PAOLETTI, *Physica*, **30**, 1942 (1964).
5. A Scattering Model for Polyphenyls and the Diffusion Parameters of Dowtherm-A, F. Seifidvash (Reactor Lab-Finland)

Among organic liquids, the polyphenyls appear to be the most resistant to the decomposing effects of the combination of high temperatures and nuclear radiations in a nuclear reactor core. Therefore, they are the most suitable of known organic compounds used in the organic-cooled, heavy-water-moderated reactors. The design of such reactors requires an accurate estimation of the thermal-neutron spectra and the diffusion parameters, all as a function of temperature, in these mediums.

To predict the thermal spectra, a model has been developed for neutron scattering by protons bound in polyphenyls, analogous to that of Neikin for water. The physical model comprises a free translator of mass 78, a hindered rotational oscillator of effective mass 21.3 at an

TABLE I  
The Diffusion Length, Diffusion Constant, and Diffusion Heating Constant for Dowtherm-A, Diphenyl and Santowax-R.

T (°C)	$\rho$ (g/cm <sup>3</sup> )	L(cm)	$D_0$ (10 <sup>5</sup> cm <sup>2</sup> /sec)	H(10 <sup>3</sup> cm <sup>2</sup> /sec)	Compound	Ref
20	1.053	4.1656	47.499	18.049	$C_{12}H_{10}O_{12}$	P. Model
20	1.053	4.190 ± .015	48.6 ± .6	17.2 ± 3.5		P. Exp.
50	1.039	4.503 ± .015	-	-		P. Exp.
80	1.014	4.7778	59.520	24.691		P. Model
80	1.014	4.782 ± .019	60.4 ± .7	27.6 ± 4.5		P. Exp.
110	0.989	5.097 ± .022	-	-		P. Exp.
140	0.963	5.4320	73.249	39.635		P. Model
140	0.963	5.422 ± .036	74.5 ± .9	34.6 ± 7.8		P. Exp.
170	0.963	5.803 ± .037	-	-		P. Exp.
200	0.908	6.1660	89.063	53.128		P. Model
200	0.908	6.205 ± .055	88.2 ± 1.6	56.4 ± 18.9	P. Exp.	
220	0.889	6.278 ± .060	-	-	P. Exp.	
24	1.056	3.9035	44.836	15.139	$C_{12}H_{12}$	P. Model
24	1.056	3.95 ± .37	48.4 ± .7	21.9 ± 2.9		2
85	0.98	4.6487	58.918	23.191		P. Model
85	0.98	4.65 ± .06	62.6 ± .8	42.9 ± 4.3	2	
106	0.97	4.8265	82.412	29.492	$C_{12}H_{12}$	P. Model
106	0.97	4.82 ± .08	65.9 ± .8	37.2 ± 4.3		2
171	0.991	5.4353	75.340	37.773	$C_{12}H_{14}$	P. Model
171	0.991	5.4580	78.309	16.336		3-4
201	0.987	5.7516	82.887	42.562		P. Model
201	0.987	5.7985	88.270	30.753		3-4
207	0.982	5.8350	84.742	44.265		P. Model
207	0.982	5.8777	89.156	19.925		3-4
232	0.943	6.1020	60.789	48.062		P. Model
300	0.89	6.8420	108.413	69.590		P. Model



energy of 0.02 eV, and two vibrational oscillators at energies 0.196 and 0.38 eV with equal masses of 2.126. The model assumes that the benzene molecule constitutes the basic dynamical unit and the differences in various polyphenyls in the reactor calculations are unimportant only in the fine structures. The sensitivity of the predictions of the model to the variations of mode parameters is investigated. The diffusion parameters were calculated by the method described by Honeck.<sup>1</sup>

The thermal-neutron diffusion length in Dowtherm-A (a eutectic mixture containing 26.5% diphenyl and 73.5% diphenyl oxide by weight) has been measured at 20, 50, 80, 110, 140, 170, 200, and 220°C. By varying the neutron absorption cross sections by the addition of trioxylene glycol borate, the neutron diffusion constant and diffusion heating constant were determined at 20, 80, 140, and 200°C. The measurement of the boron concentrations was carried out by a double-beam infrared absorption method using the characteristic absorption frequency of the B-O-B bond at 1412 cm<sup>-1</sup>.

The experiment essentially consisted of measuring the relaxation length of thermal neutrons from the thermal column of the London University reactor, in a 40 × 40 × 30-in.<sup>3</sup> aluminum tank. The negative source technique was applied using a <sup>235</sup>U fission chamber as the detector. The gastight tank was heated externally by heating blankets and the temperature was controlled to within 0.25°C. The uncertainty in the extrapolation distance for the worst case caused an error of < 0.15% in the diffusion length.

The predictions of the proposed model are in good agreement with the present results for Dowtherm-A, with experimental data<sup>2</sup> on diffusion parameters of diphenyl and with results of neutron scattering law measurements for Santowax-R.<sup>3,4</sup> The results given in the table show that as far as the reactor calculations are concerned, the benzene molecule can be taken as the basic dynamical unit for the neutron thermalization problem in polyphenyls, and that the proposed model is applicable to all the organic compounds commonly used as reactor coolants and/or moderators.

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## 6. Doppler Broadening of Resonances and Inelastic Neutron Scattering in Uranium Carbide, C. Lajeunesse (RPI), W. E. Moore (KAPL), S. N. Purohit, M. L. Yeater (RPI)

The Doppler-broadened neutron resonance cross section is given by

$$\sigma(E) = \frac{\sigma_0}{4} \int_{-\infty}^{\infty} \frac{S(K, \omega) d(\hbar\omega)}{[E_1 - E + \hbar\omega]^2 + \Gamma^2/4}$$

where  $\sigma_0$  is the peak cross section,  $\Gamma$  and  $E_1$  are the total width and resonance energy, and  $S(K, \omega)$  is the neutron scattering law. However, the gas model with an effective temperature is usually employed to evaluate  $\sigma(E)$ . For a diatomic system, one must take into account the polariza-

tion vectors in the definition of an effective temperature. This temperature will be different for each type of atom. For the  $j$ 'th atom, we have derived an effective temperature in the short collision time expansion

$$T_{j\text{eff}} = \frac{\sum_{\lambda, \alpha, \beta} (K_{\alpha} \cdot e_{\alpha}(j/\lambda))^2 (K_{\beta} \cdot e_{\beta}(j/\lambda))^2 \omega_{\lambda} \coth\left(\frac{\hbar\omega_{\lambda}}{2k_B T}\right)}{2N \sum_{\alpha, \beta} K_{\alpha} K_{\beta}}$$

where  $e_{\alpha}(j/\lambda)$  and  $e_{\beta}(j/\lambda)$  are polarization vectors, and  $K_{\alpha}$  and  $K_{\beta}$  are unit momentum transfers along  $\alpha$  and  $\beta$  directions, respectively.  $N$  is the total number of atoms in the crystal.

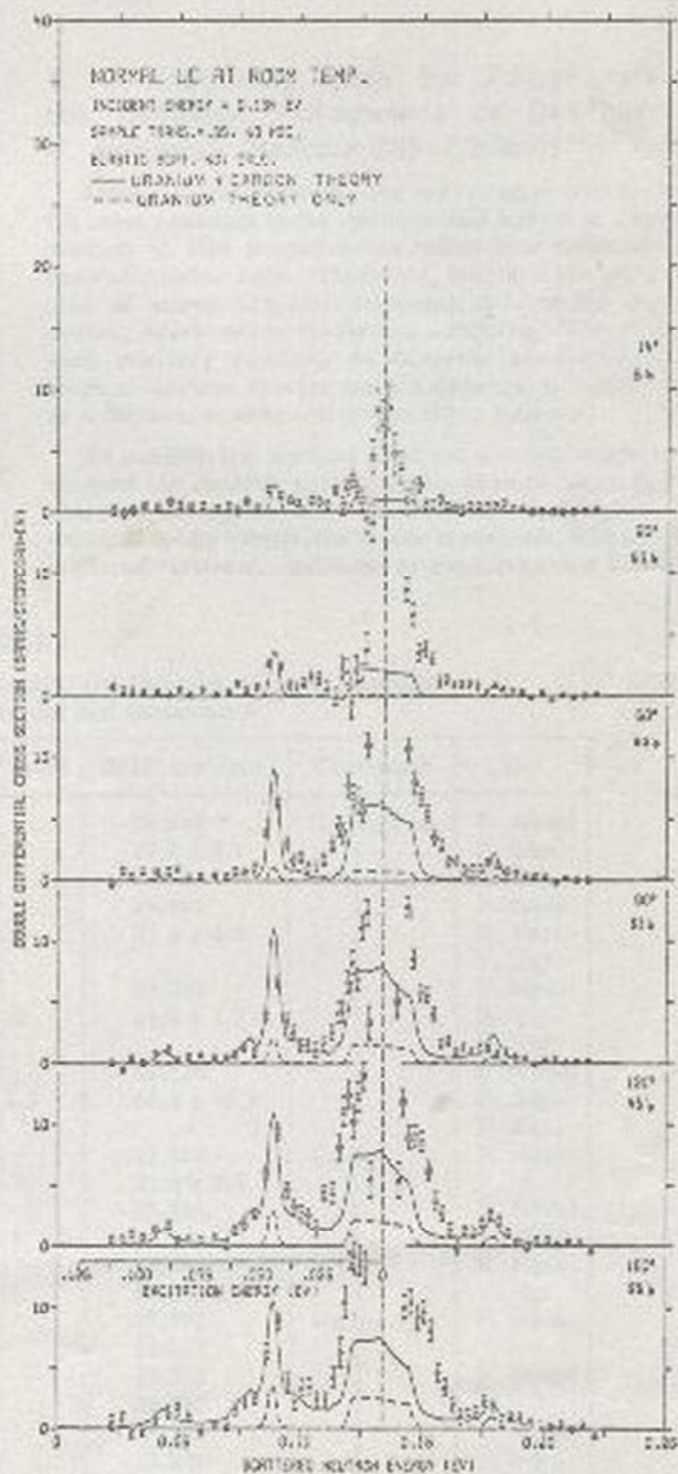


Fig. 1. Preliminary differential scattering cross sections for uranium carbide.