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1973 AND 1974

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This report presents brief summaries of the research carried out at the Israel A.E.C. laboratories during the two years 1973 and 1974.
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THEORETICAL PHYSICS AND CHEMISTRY
EFFECT OF CORRELATIONS ON THE TRANSITION TEMPERATURE AND ON THE ELEMENTARY EXCITATION SPECTRUM IN SOLID ORTHOHYDROGEN

R. Englman and Z. Friedman

The transition temperature, the nature of the ordered state below it and the elementary excitation spectrum were calculated for solid orthohydrogen subject to quadrupole-type interactions. Correlations were introduced in a way similar to that used by Onsager for polar liquids. The calculation is now consistent with the fluctuation theorem. The transition temperature obtained was 2.56\(^{0}\)K, which is very near the observed value 2.83\(^{0}\)K.

REFERENCES:
2. Onsager, L., Amer. Chem. Soc. 58, 1486 (1936)

EXCHANGE INTEGRAL AND SPECIFIC HEAT OF THE ELECTRON GAS

B. Horovitz and R. Thieberger

The system of an electron gas with positive background has been thoroughly investigated. Usually the ground state or high temperature properties were evaluated, neglecting the wide intermediate region of finite temperatures. The first order correction due to Coulomb interaction comes from the exchange term. Recently there has been an increased interest in the evaluation of the exchange term for finite temperatures\(^{(2,3)}\). These works and a previous one\(^{(4)}\) deal mainly with the expansion near T=0. Even so, the different papers disagree as to the behavior of the specific heat as T\(\rightarrow\)0.

We have derived a simple expression for the exchange term of the electron gas at any temperature T. For T\(\rightarrow\)0 we get for the specific heat:
\[ C_v \approx T \ln T + \Theta(T) \]
Using a screened potential, the result can be corrected to:
\[ C_v \approx T |\ln T| + \Theta(T) \]

REFERENCES:
4. Wohlfarth, E.P., Phil. Mag. 41, 534 (1950)
BREAKDOWN OF THE MOLECULAR FIELD APPROXIMATION FOR DIPOLAR INTERACTION

Z. Friedman and J. Felsteiner

By use of a high temperature expansion it was shown that the generally believed assumption that the molecular-field approximation should work well for long range forces is not justified for dipole-dipole interaction. This is due to the dependence of the nature of the interaction, whether ferro or antiferro, upon the direction of the vector joining every two dipoles. An effective number of nearest neighbors \( Z_{\text{eff}} \) was defined. This number is the number of nearest neighbors in the isotropic case and is quite different from that for non-isotropic interactions, such as the dipole-dipole interaction. This is the number that has to be large in order that the molecular field theories work well.

REFERENCE:

SHELL-DEPENDENT CORRELATION FUNCTIONS FOR SOLID \(^3\text{He}\)

I. Aviram and R. Thieberger

The ground state energy of solid \(^3\text{He}\) was computed by a modified Monte Carlo procedure, in which the correlation parameter for nearest neighbor pairs was assigned different values from that for more distant pairs. This results in a ground state energy which is lower by about 0.5 K than the value obtained with a single correlation parameter \(^2\).

We used two sets of (6-12) potentials. The correlation function was of Hansen's type \(^3\) with a different value of \( \lambda \). The minimum energy was obtained with Haberlandt's potential and with \( \lambda_1 = 105 \) (first shell) and \( \lambda_2 = 75 \) (all other shells). This gives -1.1 K, in good agreement with the experimental value of Pandorf and Edwards \(^4\).

REFERENCES:

* Technion, Israel Institute of Technology, Haifa
THE GENERAL CLUSTER TERM FOR SOLID $^3$He (1)
I. Zmora* and R. Thieberger

Three main approaches were developed to evaluate the ground state energy of solid $^3$He. One of these, the variational calculations approach based on the Jastrow-type trial wave function $\psi$, and using either a cluster expansion or a Monte Carlo calculation to evaluate $\langle \psi | H | \psi \rangle$, was developed by Nosanov(2), Frohberg(3), Brueckner and Thieberger(4), and Hansen and Pollock(5).

In the present work an explicit expression for the cluster terms in the expansion for $^3$He was developed. An example, using Monte Carlo integration, was given to demonstrate the use of the expression.

REFERENCES:

THE GROUND STATE ENERGY OF SOLID $^3$He (1)
E. Domany, M.W. Kirson** and R. Thieberger

The ground state energy of solid $^3$He was evaluated by means of a perturbation(2) expansion. The unperturbed hamiltonian chosen localized each atom at a given site. As such, the formalism is one of distinguishable particles. No a-priory self-consistency of the single particle potential was assumed.

The two-particle terms were evaluated with almost no numerical approximations, i.e. both center-of-mass effects and angular dependence were treated exactly. The values obtained, at each density, are reasonably close to experiment. The main deviation from experiment appears in the variation of the energy with density.

REFERENCES:

* Ben Gurion University, Beer Sheva
** Weizmann Inst. of Science, Rehovot
PHONON DISPERSION AND INSTABILITY IN LINEAR-CHAIN CRYSTALS(1)
B. Horovitz, M. Weger and H. Gutfreund*

The coupling of phonons to an electron gas with a Fermi surface consisting of two parallel planes and its effect on the stability of the lattice and on the phonon dispersion around \( 2p_v \) were considered. The phonon dispersion and the phonon spectral density distributions were calculated at zero temperature for the equidistant and the deformed lattice, and at temperatures above the transition temperature for the deformed lattice. Two excitation braches were found under certain conditions. The calculation was performed in the random-phase approximation, and the effect of vertex renormalization by summing all ladder diagrams was considered. The phonon dispersion in the distorted lattice was also treated within the framework of the Sawada model.

REFERENCE:

PEIERLS - FROHLICH INSTABILITY AND SUPERCONDUCTIVITY IN LINEAR CHAIN CRYSTALS(1)
H. Gutfreund*, B. Horovitz and M. Weger

The transition to insulating or superconducting states in linear chain systems was considered in relation to the recently observed metal-to-semiconductor transition(2,3) in TTF-TCNQ crystals. A relation between \( T_c \), the Peierls transition temperature \( T_p \), and the electron-phonon coupling strength was derived using the RPA and a simplified form of the strong coupling equation for \( T_c \). It was argued that in principle one can have either \( T_p > T_c \) or \( T_c > T_p \). The maximum value of \( T_c \) was found to be related to the unperturbed phonon frequency. Thus, in order to get a high value of \( T_c \), the electrons must be coupled to phonons possessing a high frequency, such as the stretching vibrations of the CN and CC bonds. The coupling strength between these bond vibrations and the electrons was estimated and found to be sufficiently large to make it possible in principle to obtain values of \( T_c \) of the order of 50\(^0\)K.

REFERENCES:

*Hebrew University, Jerusalem
ONE PHONON VERSUS MULTIPHONON ABSORPTION IN SMALL IONIC CRYSTALS\(^1\)

R. Ruppin

Some recently published experimental absorption curves of small crystallites of NaI, KI and MgO were shown to be in qualitative agreement with calculated absorption spectra of small spheres. Although the calculation allows for resonant, one-phonon absorption only, it reproduces all the main features of the experimental data. It was shown that allowing for multiphonon processes has a very small effect on the calculated spectra. It follows that measurements on small samples are not a sensitive tool for obtaining information about multiphonon processes in the Reststrahlen region.

REFERENCE:
1. Ruppin, R., Phys. Status Solidi (b) 50, 65 (1973)

OPTICAL PROPERTIES OF A PLASMA SPHERE\(^1\)

R. Ruppin

The classical theory for the scattering and absorption of electromagnetic radiation by a homogenous isotropic sphere was extended so as to apply to a sphere in which dispersive plasma oscillations exist. Computations performed for small metallic spheres predict the appearance of an absorption structure in the frequency region just above the plasma frequency, and a shift of the main plasma resonance towards the high frequency side.

REFERENCE:

MOLECULAR PHOTODISSOCIATION\(^1\)

S. Mukamel and J. Jortner*

A quantum mechanical model was developed for direct photodissociation and for predissociation of polyatomic molecules in terms of a sequential decay scheme involving multiple coupled continua, where each continuum corresponds to a different internal vibrational state of the fragments. The coupling matrix elements between the "initial" state and the continuum states are in general determined by the appropriate vibrational overlap factors for the polyatomic radical, while intercontinua coupling for a triatomic molecule occurs only between adjacent vibrational continua. The time evolution of the system was

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Fig. 1
Results of the model calculation for the vibrational distribution of CN($^2\Sigma$) radicals compared with the experimental data of Mele and Okabe\(\textsuperscript{2}\).

(a) ICN  (b) BrCN
handled by the Green's function method. Explicit theoretical expressions for the final vibrational distribution of the fragments in the photofragmentation of linear triatomic molecules were derived. The final distribution is determined by the initial coupling to the different continua and by a wave matrix which couples the various dissociative channels. The wave matrix was evaluated for some simple realistic models for the intercontinuum coupling. The available experimental data (2) for the vibrational distribution of the CN(B^2E) radical resulting from photodissociation and predissociation of XCN molecules are well accounted for in terms of our theory; see Fig. 1.

REFERENCES:

RESONANCE FLUORESCENCE INVOLVING OPTICALLY ACTIVE CONTINUA
S. Mukamel and J. Jortner

We have utilized the T matrix formalism of scattering theory for the study of the cross sections specifying optical absorption, resonance fluorescence elastic photon scattering, resonance Raman scattering and photodissociation for molecules undergoing direct photodissociation or predissociation into a continuum, which carries oscillator strength from the ground state. We have demonstrated that for the special case of radiative interactions with a single molecular continuum explicit expressions can be derived for the Green's functions and for the reaction operator, incorporating radiative interactions with one photon states to infinite order. From the complete solution for elastic photon scattering from a dissociative continuum we conclude that the direct radiative corrections are of the order of the "radiative Lamb shift" for the continuum states, and are negligible. The elastic photon scattering cross sections can be expressed in terms of a complex Hilbert transform of the Franck-Condon transition density, while the absolute photon scattering quantum yield is ~ 10^-7. This treatment has been extended for the study of resonance Raman scattering from a dissociative continuum, where the scattering cross sections can be expressed in terms of absolute squares of complex Hilbert transforms of the product of two Franck-Condon vibrational overlaps for bound-continuum transitions. No selection rules for the final vibrational state are exhibited.

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Finally, we derived a general solution for photon scattering for a discrete molecular level coupled to an optically active dissociative continuum (2).

The absorption cross section is finite at the interference dip, being determined by the interference function for the continuum states. The quantum yield for resonance fluorescence exhibits a sharp maximum reaching a value of unity at the interference dip where the quantum yield for dissociation vanishes.

Typical results for the various cross sections in the Fano problem are given in Fig. 2.

![Fig. 2](image)

**Fig. 2**

Photon absorption ($\sigma_a$) and scattering ($\sigma_s$) cross sections for the interference (Fano) problem (2). $\epsilon$ and $q$ are the reduced parameters defined by Fano whereas $Y_r$ is the photon scattering quantum yield. $\sigma_a^0$ and $\sigma_s^0$ are the cross sections in the absence of the discrete level.

REFERENCES:

SEQUENTIAL DECAY INVOLVING MULTIPLE CONTINUA

S. Mukamel and J. Jortner

Green's function method was used to derive an explicit solution for the problem of sequential decay involving multiple continua with constant coupling between adjacent continua. This model system is applicable for theoretical studies of dynamics of photodissociation, predissociation and electronic quenching of polyatomic molecules. Another possible application involves the vibrational excitation of molecules by electron impact which proceeds via the formation of an intermediate negative ion.

The model results in an exponential decay of the initially prepared state, however, there is a retardation of the decay rate due to interference effects between the final coupled channels.

Explicit expressions were developed for the final distribution among the various open channels $P_V(\omega)$ where $V$ is the channel index. Figure 3 gives

![Graph showing vibrational distributions for a sequential decay scheme. The various curves differ by the intercontinuum interference parameter $|\beta|$](image)

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some typical distributions, \( P_v^{(\beta)} \) differing by the value of the dimensionless interference parameter \( |\beta| \) which is proportional to the coupling strengths between the final channels and their density of states. We assume that the initial state is coupled to the \( V=0 \) channel (and so for \( |\beta|=0 \) we have \( P_v^{(\beta)}=\delta_{V,0} \)).

Partitioning between the final channels becomes wider as \( |\beta| \) increases. For large \( |\beta| \) we see that the distributions need not be smooth which provides a possible explanation for the experimental results concerning vibrational distribution of diatomics due to electronic-to-vibrational energy transfer from a metastable atom (2).

The results of this model differ appreciably from those of the semiclassical half collision model (3,4) recently proposed for describing vibrational distribution among the products of photodissociation of triatomics. However, the semiclassical Poisson distribution is obtained as a limiting case of our model.

REFERENCES:

ON THE APPLICATION OF SEPARABLE POTENTIALS IN THE DESCRIPTION OF RESONANCE FLUORESCENCE

S. Hukamel and J. Jortner

Molecular photodissociation and photon scattering from a photodissociating system involve direct coupling of a photon continuum to an intramolecular continuum (or a set of coupled continua). The applicability of "separable potentials" for the quantum mechanical description of these processes was considered. Such intercontinua interaction potentials of the form \( \langle n|V|m\rangle = V_1(n) V_2(m) \) were extensively used in nuclear scattering theory (2).

The electromagnetic interaction is formally nonseparable, since it explicitly contains the angle between the molecular transition dipole and the photon polarization; however by invoking the Condon approximation it may be

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brought into a separable form. It was explicitly shown that for diatomics, in the axial recoil approximation \(^{(3)}\) the separability is achieved without adopting the Condon approximation.

REFERENCES:

COMPLETE SOLUTION OF THE HASEGAWA COUPLED EQUATIONS OF MOTION: THE PROBLEM OF RELAXATION DESTINATION
G. Dublon and D. Davidov*

Recent electron spin resonance (ESR) measurements of \(\text{Gd}_{x}\text{Lu}_{1-x}\text{Al}_2\) intermetallic compounds indicate the presence of "bottleneck" and "dynamic" effects in the relaxation mechanism \(^{(1)}\). This is due to the fact that the electron gas spin system is not an infinite heat reservoir, and due to the proximity of the field of resonance of the paramagnetic ions and the conduction electrons. An attempt to interpret this behavior requires a complete solution of the Hasegawa-type equations of motion \(^{(2)}\), which describe the dynamic behavior of coupled spin systems. This is especially so because of the non-linearity of the ESR linewidth vs. temperature curve observed for very low Gd concentrations (50 ppm) at low temperatures (0.6\(^{\circ}\)-1.5\(^{\circ}\)K), even in the absence of a "bottleneck" effect.

Hasegawa distinguishes between relaxation towards a time-averaged thermal equilibrium and towards an instantaneous local equilibrium. Ambiguity is, however, present concerning the relaxation destination, as authors disagree on whether the relaxation is towards a time-averaged or an instantaneous local field \(^{(3)}\).

By solving the Hasegawa equations, a good fit with the experimental results was obtained. The \(\text{Gd}_{x}\text{Lu}_{1-x}\text{Al}_2\) system was further solved for a relaxation both towards a time-averaged and a local instantaneous field.

Qualitatively, the temperature dependence of the ESR linewidth and "g-shift" was found to be independent of the relaxation destination.

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Quantitatively, a measurable change in the linewidth and 'g-shift' is predicted at low temperatures and high Gd concentrations, as the relaxation destination is varied.

REFERENCES:

NON-LINEAR BEHAVIOR OF SOLUTIONS ILLUMINATED BY A RUBY LASER
A. Zunger and K. Bar-Eli

The simultaneous non-linear time-space equations governing the light intensity and electronic molecular level population in laser-illuminated media were numerically solved for a postulated energy level scheme. The purpose was to obtain a quantitative fit to a series of independent measurements at high light intensities, via a chosen energy level scheme and assumed decay-time rate constants. In a previous paper(2) cryptocyanine dye was chosen as an example, while here we treated other dyes that are important for passive Q-switching, namely phthalocyanine (H.Pc) and chloro-aluminium-phthalocyanine (Cl-A-Pc). The experimental data for these materials exist in the literature on the following subjects:

a) absorbance as a function of light intensity for various concentrations
b) fluorescence intensity (both from lowest excited and from second excited states) as a function of laser intensity
c) time profile of both fluorescence emissions for low and high intensities
d) fluorescence quantum yield at saturation limit and at lower intensities
e) time dependent transmission curves
f) narrowing of the outcome laser time profile as a function of its initial intensity after transmission through the cell
g) decay of fluorescence through the triplet
h) double-beam experiments

A computer program was developed which accepts as input an initial guess for a model of molecular energy levels and the rate constants coupling them. It then calculates the various populations of these levels as a function of time and spatial location and computes the expected results for the experiments listed

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above. The time profile of the input laser is also given as input. The program then seeks a minimal energy level scheme and varies the input rate constants to get a best fit. A very good fit was obtained for a 4-level scheme for $H_{2}$PC and Cl-A-PC and the results are in general agreement with previous suggestions for these materials.

REFERENCES:

SMALL PERIODIC CLUSTER CALCULATION ON POINT DEFECT PROBLEMS IN HEXAGONAL LAYERED SOLIDS\(^{(1)}\)

A. Zunger

A model was proposed for discussing deep defect levels in covalent solids, based on the representation of one-electron energies of the crystal by the eigenvalue spectrum of a small periodic cluster of atoms. The model previously proposed for treating band structure of perfect hexagonal solids\(^{(2)}\) was extended to treat defect problems. A defect atom (impurity or vacancy) is surrounded by several shells of atoms arranged according to the perfect crystal symmetry and periodic boundary conditions are imposed on the surface. The eigenvalue spectrum is solved by applying semilemperical MO-LCAO minimal-basis methods. In the absence of the perturbation imposed by the defect atom, the eigenvectors are analyzed according to the perfect lattice wavevectors and the band structure is obtained, while in the defect problems the eigenvectors are analyzed according to the irreducible representations of the cluster containing the defect. Self-consistent LCAO methods applied to this cluster account for the charge redistribution induced by the defect. Lattice relaxations around the defect site are simply introduced by solving for the eigenvalue problem of a relaxed cluster. Three experimentally well known defect structures in hexagonal lattices were treated: a) nitrogen vacancy in boron nitride, b) carbon vacancy in graphite, c) substitutional boron impurity in graphite. In each case the character of the defect levels was investigated as to their charge distribution, degree of localization and distance from the edges of the valence and conduction bands. The results were shown to be in quantitative agreement with EPR, Hall effect and thermoluminisance measurements.

REFERENCES:
MOLECULAR CALCULATION OF ELECTRONIC PROPERTIES OF LAYERED CRYSTALS: TRUNCATED CRYSTAL METHOD (1)

A. Zunger

A truncated crystal approach was suggested for the study of electronic properties of perfect and defect two-dimensional layered solids, such as boron nitride (BN) and graphite. The method is characterized by treating a finite number of atoms arranged spatially according to a given crystalline space group by MO-LCAO methods and obtaining the convergence limit of its eigenvalues as a function of cluster size. Self-consistent semiempirical approximations to the Hartree-Fock-Roothan equations were used (2). The method was applied to hexagonal BN as an illustrative example. The work function, band gap, band-to-band transition energy, various band widths, crystal cohesive energy, equilibrium interatomic distance as well as atomic charge distributions, were calculated and found to agree favorably with experimental spectral, thermo-chemical, ESCA, NQR and crystallographic data. Frenkel pair formation energy was then calculated by the same method for BN and graphite. The results for graphite were found to agree favorably with radiation damage data while the results for boron nitride were suggested as a prediction. Recent electron beam radiation damage experiments carried out in our laboratory indicate favorable agreement with these calculated results. Localized defect problems such as nitrogen vacancies in BN were treated by the same approach. The charge distribution obtained for the defect level and its separation from the conduction band were found to agree with EPR and thermoluminescence experiments (3).

The main advantage of the method lies in the fact that it permits the treatment of both perfect lattice band structure and point defect problems within the same level of approximation. It was shown however that surface effects introduced by the dangling bonds significantly perturb the perfect band states unless a sufficiently large cluster is chosen.

REFERENCES:
MOLECULAR CALCULATION OF ELECTRONIC PROPERTIES OF LAYERED CRYSTALS - SMALL PERIODIC CLUSTER (SPC) APPROACH TO PERFECT LATTICES OF GRAPHITE AND BORON NITRIDE

A. Zunger

Small periodic clusters (18-32 atoms) of two-dimensional hexagonal structures of D$_{3h}$ and D$_{6h}$ point symmetry (such as boron nitride (BN) and graphite, respectively) were shown to possess some high-symmetry energy points in the crystalline Brillouin zone, when the eigenvalue problem is formulated by the tight binding scheme for finite structures. Semi-empirical self-consistent all-valence electron LCAO methods were used to obtain the eigenvalues and wave functions of such periodic clusters both for graphite and BN. The results agree both with extended basis orthogonalized plane wave (OPW) calculations and with experimentally adjusted tight-binding band structure. The importance of introducing self-consistency in the band structure calculation of heteropolar crystals (such as BN) was demonstrated. Properties that are difficult to evaluate by conventional tight-binding approaches employing free atom potentials, such as cohesion, interatom distance dependence of the band structure and degree of ionicity, were calculated by applying well known quantum chemical techniques to the small periodic cluster problem.

REFERENCE:

BAND STRUCTURE OF HYDROGEN BONDED HF CRYSTALS

A. Zunger

Hydrogen-bonded solids pose interesting problems with regard to their electronic properties in the condensed phase, relative to the properties of the molecules forming them. In particular, HF crystals exhibit marked differences in the bonding structure relative to isolated dimers and single molecules.

A self-consistent band structure calculation was attempted, using the previously suggested small periodic cluster approach. A periodic cluster containing up to 22 HF units, arranged according to the known space group, was taken. The eigenvalues for this cluster were computed, using the INDO approximation for the hamiltonian matrix elements. The theoretical conformation of the solid was established by minimizing the total energy as a function of geometry. This stable conformation is close to the crystallographically known structure. The band structure obtained exhibits marked differences (wider bands and greater
shift of energies at the zone boundaries relative to the isolated HF spectrum) when compared with non-selfconsistent calculations performed recently by Bassani et al.\(^{(3)}\). Further calculations of impurities in HF crystals and theoretically determined force constants to be compared with empirical lattice dynamical calculations are in progress.

REFERENCES:

SEMIEMPIRICAL LCAO CALCULATIONS OF ELECTRONIC AND DYNAMICAL PROPERTIES OF $\alpha$ AND $\gamma$ NITROGEN CRYSTALS AND NITROGEN AGGREGATES\(^{(1)}\)

A. Zunger

Semiempirical LCAO methods (extended Huckel, iterative extended Huckel and INDO) were examined as possible simple starting points for constructing solid state interaction potentials for nonbonded interactions from molecular wave functions. These methods were applied to calculate the cohesion energy and lattice equilibrium unit cell dimensions for $\alpha$ and $\gamma$ nitrogen crystals, the lattice optical mode frequencies at $\mathbf{q}=0$ of $\alpha$-N\(_2\), the electronic Davydov splitting of the molecular $^{1}\Pi_8$ state in $\alpha$-N\(_2\) and the stability of molecular-ion aggregates. Reasonable agreement was obtained with extended Huckel and iterative extended Huckel methods, while INDO usually yielded poor results. The possibility of excimer formation in nitrogen was considered in light of these calculations. It was concluded that semiquantitative results can be obtained with these methods when they include the gross features essential for description of crystal nonbonded interactions, such as full overlap interactions, approximate magnitude of molecular permanent quadrupole moment, orthogonality corrections and self-consistent charge transfer. However, when more accurate results are required, \textit{ab-initio} methods cannot be avoided.

REFERENCE:

ELECTRONIC PROPERTIES OF COMPRESSED MOLECULAR HYDROGEN CRYSTALS\(^{(1)}\)

A. Zunger

A truncated crystal model was applied to the Pa3 molecular phase of solid H\(_2\). The INDO and iterative extended Huckel (IEXH) methods were used as LCAO approximations for obtaining eigenvalues. Various electronic properties were computed as a function of the cluster size (up to 155 atoms with 1S
orbital on each atom) by diagonalizing the electronic secular equations for various clusters. The properties investigated were:

a) convergence of the band gap, ionisation potential and bandwidth with the number of atoms in the finite cluster. At the convergence limit, these properties were examined as a function of crystal density.

b) the repulsive part of the intermolecular interaction potential as yielded by LCAO methods.

c) the electronic Davydov splitting of the lowest excited singlet as well as its density dependence and the joint density of states in the neighborhood of this excited state.

d) defect states arising from H atom or N₂ impurities in solid hydrogen. The impurity levels were investigated with regard to their charge distribution and stabilization by lattice relaxations.

REFERENCE:

ENERGY LEVELS AND QUADRUPOLE COUPLING CONSTANTS OF A TRUNCATED CRYSTAL OF Be
S. Goren, G. Erez, and J. Pelleg

An attempt was made to use the truncated crystal approach in calculations of localized properties of beryllium. A crystal of 21 Be atoms was chosen and the geometry was fixed according to the crystallography of Be. The INDO\textsuperscript{(1)} approximation in the context of the LCAO-MO method was used. The calculated properties do not agree with experimental data. It was concluded that the INDO method is not suitable for such calculations in metals, most probably because overlapping between neighboring atoms is neglected.

REFERENCE:

OPTICAL PROPERTIES OF HEXAGONAL BORON NITRIDE\textsuperscript{(1)}
A. Zunger, A. Katzir and A. Halperin

Optical absorption, reflectivity and photoconductivity in the range near UV (1900-4000 \AA) of a thin film of hexagonal boron nitride were measured. The main absorption peak was observed at 6.2 eV. A sharp fall at about 5.8 eV was attributed to the direct band gap. The temperature dependence of the band gap was found to be less than 4x10\textsuperscript{-5} eV/deg.

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Self-consistent tight binding band structure calculations were performed on a two-dimensional hexagonal crystal model, using Hamiltonian matrix elements calculated by semiempirical LCAO methods for clusters of atoms having the hexagonal crystal structure. The calculated value for the band gap of HBN was in reasonably good agreement with the experimental value obtained in the present work, as well as with values reported earlier from electron energy loss and photoelectron emission measurements.

The calculations also predicted a very small change in the band gap with temperature, in agreement with the experimental observations.

REFERENCE:

CALCULATION OF STRUCTURAL PROPERTIES AND VIBRATIONAL FREQUENCIES OF \( \alpha \)- AND \( \gamma \)-N\(_2\) CRYSTALS

A. Zunger and E. Huler

Current lattice dynamical calculations on atomic solids have been recently extended to molecular crystals. In this research, we critically examined the various approximations involved in these calculations, namely the effect of zero-point-energy on phonon frequencies (via a self-consistent calculation), the effect of the residual forces and torques on the spectrum and the effects of truncated lattice sums on the equilibrium crystal structure. Numerical computations were performed on the two structural phases of solid nitrogen - the \( \alpha \) cubic phase and the \( \gamma \) tetragonal phase. Using the experimental intramolecular potential and a phenomenological intermolecular interaction we computed the phonon dispersion curves, intramolecular modes, cohesive energy, equilibrium unit cell parameters, Grüneisen mode parameters, P-V data, \(^{14}\text{N}/^{15}\text{N}\) isotope effects, and the second virial coefficient of the fluid. These calculated properties are in good agreement with Raman and IR results, X-ray data and thermochemical measurements. The \( \alpha \) to \( \gamma \) structural phase transition is however not revealed by the potential employed.

REFERENCE:
LATTICE DYNAMICS OF SOLID $\alpha$- AND $\gamma$-$N_2$ CRYSTALS AT VARIOUS PRESSURES

E. Huler and A. Zunger

A previously published interaction potential between $N_2$ molecules was utilized to compute the lattice mode frequencies of solid $\alpha$- and $\gamma$-$N_2$ at the equilibrium crystal structure corresponding to various pressures. Dispersion curves and density of states were determined. These were then used to calculate the lattice heat capacity, Grüneisen mode parameters throughout the Brillouin zone, linear thermal expansion coefficient, Debye temperatures and root mean square amplitudes of vibrations. Wherever comparison with experimental data was possible, good agreement was obtained.

REFERENCE:

INCORPORATION OF INTER- AND INTRAMOLECULAR FORCES IN THE CALCULATION OF CRYSTAL PACKING AND LATTICE VIBRATIONS

E. Huler and A. Warshel

A general method for the simultaneous calculation of the effect of inter- and intramolecular forces on crystal packing and lattice dynamics was developed. The crystal potential is analytically represented as a function of the $3n$ Cartesian coordinates of the $n$ atoms in the asymmetric unit and the 6 unit cell parameters. The equilibrium geometry and the lattice vibrations are consistently derived from the same crystal potential. The applicability of the method for both rigid and flexible molecules was demonstrated by calculations of benzene, biphenyl and $8$-ionolydene crotonic acid. The computer programs developed in this work are available.

REFERENCE:

VIBRONIC STRUCTURE OF CRYSTALLINE ETHYLENE

P. Dauber**, M. Brith**, E. Huler and A. Warshel*

The vacuum UV spectrum of solid ethylene was measured and the vibronic structure of the $\pi \rightarrow \pi^*$ transition calculated. The strong progression which

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**Bar Ilan University, Ramat Gan
appears in the spectrum of the crystal was shown to be due, as in the spectrum of the gas, to a large torsional distortion of the equilibrium of the molecule upon electronic excitation. The lengthening of the C-C bond on the V state also contributes to the vibronic structure. The calculations show that the crystal forces are weak and do not hinder the distortion of the molecule in the crystal. Thus ethylene serves as a model for the weak coupling case of excitations in molecular crystals.

REFERENCE:

ABSENCE OF ISOTOPIC STABILIZATION IN JAHN-TELLER SYSTEMS
B. Halperin and R. Englman

An isotopic mass change in the neighborhood of a Jahn-Teller ion was shown to have effects equivalent to that of an asymmetric potential whose strength is proportional to the Jahn-Teller stabilization energy and to the square of the relative mass change. A situation like this arises in the superhyperfine structure measurements on the EPR spectra of Ni$^{3+}$ in isotopically labeled crystals of MgO, which have recently been reported. Because of the smallness of the square of the relative mass change for $^{17}$O, the isotope effect is not competitive with commonly occurring random strain fields.

REFERENCES:

EFFECTIVE-HAMILTONIAN APPROACH TO JAHN-TELLER COUPLING OF IMPURITIES IN CRYSTALS
R. Englman and B. Halperin

The problem of an impurity ion subject to linear Jahn-Teller coupling with vibrational modes of the crystal was reconsidered. A trial ground-state wavefunction was postulated in which one linear combination of vibrational modes behaves as though subject to a molecular Jahn-Teller effect while the rest are decoupled from the electronic states. The linear combination was selected by a variation of the ground-state energy of the system.

REFERENCE:
REDUCTION FACTORS FOR THE JAHN-TELLER EFFECT IN SOLIDS\(^{(1)}\)
B. Halperin and R. Englman

The degeneracy of the vibronic ground state of a Jahn-Teller coupled system is known to remain the same as that of the original electronic state, and the effects of the vibronic coupling are manifested by the reduction in the values of various perturbations which split the ground state multiplet. We report on the distinction, in the linear Jahn-Teller effect of an electronic \(E\) state, between coupling with one set of doubly-degenerate vibrational modes and coupling with several such sets of different frequencies (the multimode Jahn-Teller effect) as is the case for an impurity in a solid. Whereas the combination of the reduction factors \(2q-p\) is exactly unity in the former case, it is shown to be less than unity in the latter. Also, the value of \(q\) may decrease below one half, which is its minimum value obtained for linear coupling with only one pair of modes.

REFERENCE:

TWO-FREQUENCY DESCRIPTION FOR THE JAHN-TELLER COUPLING OF IMPURITIES IN SOLIDS\(^{(1)}\)
B. Halperin and R. Englman

A variational treatment was applied to the multimode Jahn-Teller effect of an impurity ion in a crystal. The case treated was an electronic doublet. For vibronic coupling to modes in a sufficiently narrow frequency range a single-effective-frequency description was shown to be adequate for the ground state of the system. For coupling to modes whose frequencies are very different (e.g. acoustic and optical phonon modes) a two-effective-frequency description is preferred. Expressions were derived for the best (in the variational sense) frequencies and coupling strengths of the effective modes. A solution was obtained for the linear coupling problem between an electronic doublet and two vibrational doublets, in the limit of strong coupling. The reduction factors for external perturbations and the coupling to strain were evaluated.

REFERENCE:
ASYMMETRIC DISSOCIATION OF A SYMMETRIC MOLECULE: PHOTOFragmentation Dynamics of Cd(CH₃)₂

M. Tamir, U. Halavee and R.D. Levine

A theoretical analysis of the dissociation of energy-rich triatomic molecules showed that asymmetric dissociation is expected to be the major decay mode. Both experimental and computational (classical trajectories) results for the photofragmentation of Cd(CH₃)₂ are in accord with the theoretical analysis.

REFERENCE:

QUANTUM MECHANICAL TREATMENT OF THE COLLINEAR H⁺+H₂ SYSTEM. I. THE UNCOUPLED SYSTEM

Z.H. Top and M. Baer

A fully converged close coupling study of the collinear (H⁺+H₂) system on the lowest potential energy surface was performed. The surface was derived by the DIM7.0 (diatomic in molecules zero overlap) method. Transition probabilities for the reactions

H⁺ + H₂ (v = 0, 1) → H₂(v') + H⁺ ; \quad v' = 0, ..., 7

were given for a number of total energies in the range from 1 eV to 3 eV. It was found that for this energy region the transition v=0 → v'=0 is the most preferential. This fact leads us to believe that addition of the upper surface will have a minor effect on the calculated probabilities of transitions from v=0 in the above-mentioned energy range.

REFERENCE:

* Weizmann Institute of Science, Rehovot
** This work is part of a study for the Ph.D. Degree to be presented by Z.H. Top to the Feinberg Graduate School, Weizmann Institute of Science, Rehovot.
COLLINEAR QUANTUM MECHANICAL CALCULATIONS OF THE He+H₂ PROTON TRANSFER REACTION

M. Baer and D.J. Kouri

Exact quantum mechanical results for collinear He + H₂⁺ → H + HeH⁺ reactive collisions were obtained for the (total) energy range of 0.93 eV to 1.4 eV. The H₂⁺ initial vibrational states include v = 0 through v = 5. The diatomics-in-molecules semi-empirical surface of Kuntz was used in the computations. Except for a short range of energies, the calculated reaction probabilities for H (v = 0) are larger than those of excited H₂⁺.

REFERENCE:

THE COLLINEAR Cl+XY SYSTEM (X,Y=H,D,T). A COMPARISON BETWEEN QUANTUM MECHANICAL, CLASSICAL AND TRANSITION STATE THEORY RESULTS

M. Baer, U. Halavee and A. Persky

Exact quantum mechanical (QM) and classical (CL) transition probabilities for the Cl+XY (X,Y=H,D,T) collinear system were compared. The calculations were performed using a semiempirical LEPS surface. The main features considered were tunneling and threshold behavior for both the ground state and the first excited state of the hydrogen molecule. Kinetic isotope effects were calculated in three different ways, using (a) QM transition probabilities, (b) CL transition probabilities, and (c) transition state theory (TST-1D). Tunneling coefficients k_QM/k_CL and k_QM/k_TST were calculated. A brief comparison with experimental data was also made.

REFERENCES:

EXACT QUANTUM MECHANICAL STUDY OF KINETIC ISOTOPE EFFECTS IN THE COLLINEAR REACTION Cl+H₂ → HCl+H. THE H₂/D₂ AND THE H₂/T₂ ISOTOPE EFFECTS

A. Persky and M. Baer

Exact quantum mechanical probabilities for the collinear reaction of chlorine atoms with H₂, D₂, and T₂ in their ground and first vibrational
excited states were calculated for a semiempirical LEPS potential energy
surface. These probabilities were used to calculate the kinetic isotope
effects \( \frac{k_{\text{Cl}+\text{H}_2}}{k_{\text{Cl}+\text{D}_2}} \) and \( \frac{k_{\text{Cl}+\text{H}_2}}{k_{\text{Cl}+\text{T}_2}} \) which were compared with experi-
mental data and with results of transition state theory calculations. The
effect of the vibrational excitation of the hydrogen molecules on the rate of
their reaction with chlorine atoms was also studied.

REFERENCE:

AN EXACT QUANTUM MECHANICAL STUDY OF THE ISOTOPIC COLLINEAR REACTIVE SYSTEMS
\( \text{H}_2+\text{Cl} \) AND \( \text{D}_2+\text{Cl} \) \(^{(1)}\)
M. Baer

An exact quantum mechanical study was performed on the collinear reactive
systems \( \text{H}_2+\text{Cl} \) and \( \text{D}_2+\text{Cl} \). Using an LEPS surface with a barrier height of
0.33 eV, the reactive transition probabilities were derived. Isotopic effects,
threshold effects, effects of opening of new states and the influence of the
initial state were considered to some extent.

REFERENCE:

ISOTOPIC REACTIVE SYSTEMS \( \text{H}+\text{Cl}_2 \) AND \( \text{D}+\text{Cl}_2 \). A QUANTUM MECHANICAL TREATMENT
OF THE COLLINEAR ARRANGEMENT\(^{(1)}\)
M. Baer

An exact quantum mechanical study was performed of the collinear reactive
systems \( \text{H}+\text{Cl}_2 \) and \( \text{D}+\text{Cl}_2 \). The surface applied in this work is a LEPS poten-
tial surface originally employed by Polanyi and co-workers\(^{(2,3)}\). The main
results are: (a) a strong population inversion is found, the most populated
levels being \( v = 4 \) for the HCl product and \( v = 5 \) for DCl; (b) the initial
vibrational state has very little influence on the rate of the reaction but
strongly affects the final vibrational distribution of the product; (c) the
two isotopic systems behave very similarly (as a function of relative energy);
(d) at all points where there are classical trajectory data there is a broad
agreement with the quantum results.

REFERENCES:
2. Anlauf, K.G., Kuntz, P.J., Maylotte, D.H., Pacey, P.D., and Polanyi, J.C.,
   Discuss. Faraday Soc. 44, 183 (1967)
3. Anlauf, K.G., Hane, D.S., MacDonald, R.G., Polanyi, J.C., and Woodall, K.B.,
   J. Chem. Phys. 57, 1561 (1972)
TRANSLATIONAL SPECTRUM DUE TO TERNARY COLLISIONS IN PURE RARE GASES\textsuperscript{(1)}
S. Weiss

A simplified model was used to predict the spectral region in which the translational absorption spectrum due to ternary collisions in a pure monoatomic gas is to be expected and its general shape. Spectra predicted for Ar at various temperatures and for Kr and Xe at one temperature are shown in Fig. 4. Analytical expressions were obtained for the absorption coefficient and for the integrated intensity.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{Spectra due to ternary collisions in pure rare gases as calculated from our model. The dipole moment range has been assumed to be $\rho = 0.5$ Å and its strength $\nu_0 = 0.01$ debye for all the cases shown; the density is one amagat unit.}
\end{figure}

REFERENCE:

DIPOLAR MOMENT OF INTERACTING RARE-GAS ATOMS\textsuperscript{(1)}
E. Bar-Ziv and S. Weiss

The translational absorption spectra of He-Ar and Ne-Ar were analyzed with a hard-sphere potential to obtain the explicit dependence of the interaction dipoles on interatomic distance (Fig. 5). The dipoles were found to consist of a short-range part varying almost exponentially with the distance...
and of a long-range part which varies more slowly. $\mu_{\text{He-Ar}}(r)$ exhibited an unexpected maximum at small distances.

REFERENCE:

LOW TEMPERATURE THEORIES OF MAGNETO-ELECTRIC EFFECTS$^{(1)}$
H. Yatom and R. Englman

Previous work was extended to incorporate more refined de-coupling approximations in the Green function theories for two sublattice antiferromagnets. These theories have strict validity only in the temperature region much below the Neel temperature; however, by considering the ratio of the magneto-electric susceptibility to the sublattice magnetization, the reliability of the theories was extended, even up to the critical region. Also, comparisons of this ratio with experimental results (for Cr$_2$O$_3$) permits discrimination between alternative mechanisms.

REFERENCE:
SOME NEW THERMODYNAMIC INEQUALITIES FOR MAGNETIC AND DIELECTRIC MATERIALS\(^{(1)}\)
H. Yatom

Systems consisting of permanent magnetic dipoles (para-, ferro- or antiferro-magnetic), which can also be, additionally or alternatively, electrically ordered were considered. The conditions for a minimum of the free energy function at thermodynamic equilibrium imply some inequalities. These are equivalent to setting upper limits for the (forced) magnetostriction, the electrostriction as well as for the magnetoelectric susceptibility. For the case of the magnetoelectric susceptibility this was previously shown\(^{(2)}\) by the method of "thermodynamic perturbation theory". However, our derivation is more general.

We have derived the following inequalities

\[ a) \quad \chi_M^K > \left( \frac{1}{V} \frac{\partial V}{\partial H} \right)^2 \_{H,T} \]

\[ b) \quad \chi_E^K > \left( \frac{1}{V} \frac{\partial V}{\partial E} \right)^2 \_{P,T} \]

\[ c) \quad \chi_M \chi_E > (\chi_{ME})^2 \]

where \( \chi_M \), \( \chi_E \) and \( \chi_{ME} \) are the magnetic, electric and magnetoelectric susceptibility, respectively; \( K \) is the compressibility defined as \(- \frac{1}{V} \frac{\partial V}{\partial P} \); \(- \frac{1}{V} \frac{\partial V}{\partial H} \) and \(- \frac{1}{V} \frac{\partial V}{\partial E} \) are the (forced) magnetostriction and electrostriction coefficients, respectively.

REFERENCES:

THE CALCULATION OF INTEGRALS IN QUANTUM ELECTRODYNAMICS
Y. Shima

The calculation of matrix elements in quantum electrodynamics of processes of the fourth order and higher is known to be very difficult. Only in very few cases have the integrals in such matrix elements been evaluated analytically.

We have shown how to obtain analytical results in certain fourth order processes, which are related to the well known case of scattering of light by
light. The functions which appear in the final result are elementary functions and the Di-Logarithm \(^{(1)}\), which is well tabulated. In this way one can obtain a relatively simple expression for the differential cross section of the process under investigation.

These results were used to obtain total cross sections of two processes: photon splitting and photon coalescence.

**REFERENCE:**

1. Mitchell, K., Phil. Mag. 40, 351 (1949)

**LEVEL STRUCTURE OF DOUBLY IONIZED ERBIUM (Er III) \(^{(1)}\)**

N. Spector

The low levels of the four basic configurations of doubly ionized erbium \(4f^{12}(^3H_{6,5}, ^3F_4)\), \(4f^{11}(^4I_{7/2})5d\), \(4f^{11}(^4I_{7/2}, ^6I_{7/2})6p\) were found (see Tables 1-3). More than a hundred Er III lines were classified by 24 odd and 18 even levels. Values for the spin-orbit parameters obtained directly from the observed levels are \(\zeta_{6p}=3743 \text{ cm}^{-1}\), \(\zeta_{6d}=1326 \text{ cm}^{-1}\).

**TABLE 1**

<table>
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<th>Designation</th>
<th>J</th>
<th>Position (cm(^{-1}))</th>
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</thead>
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<td>7</td>
<td>55547.26</td>
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<tr>
<td>$4f^{11}(^4I_{7/2})5d1^2_s$</td>
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<td>18976.74</td>
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<td></td>
<td>5</td>
<td>29806.49</td>
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</table>
TABLE 3

Observed 4f\textsuperscript{12} levels of Er III compared with the corresponding 4f\textsuperscript{12}6s\textsuperscript{2} levels of Er I

<table>
<thead>
<tr>
<th>Designation</th>
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<th>Er III (cm\textsuperscript{-1})</th>
<th>Er I (cm\textsuperscript{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>4f\textsuperscript{12} 3\text{^H}</td>
<td>6</td>
<td>0.00</td>
<td>0.00</td>
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<tr>
<td>3\text{^F}</td>
<td>4</td>
<td>5081.79</td>
<td>5035.19</td>
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<tr>
<td>3\text{^H}</td>
<td>5</td>
<td>6969.78</td>
<td>6958.34</td>
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</table>

REFERENCE:

COMMENT ON THE GROUND-STATE CONFIGURATION OF NEUTRAL URANIUM (U I)\textsuperscript{(1)}

N. Spector

The 40 levels of the ground-state configuration 5f\textsuperscript{3}(4\text{^L})6d 7s\textsuperscript{2} of neutral uranium were calculated in intermediate coupling with seven radial parameters. A least-squares fit to 27 observed levels (rms error of 475 cm\textsuperscript{-1}, \approx 3\% of the width) resulted in new values for the radial parameters (see Table 4), predictions for the missing levels and for g factors, and percentage compositions in L-S and J-j couplings.

TABLE 4

Radial parameters for 5f\textsuperscript{3}(4\text{^L})6d 7s\textsuperscript{2} of U I

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Diagonalization (in cm\textsuperscript{-1})</th>
<th>Least squares (in cm\textsuperscript{-1})</th>
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<tr>
<td>F\textsubscript{0}</td>
<td>13600</td>
<td>13347 ± 235</td>
</tr>
<tr>
<td>F\textsubscript{2}</td>
<td>110</td>
<td>121 ± 31</td>
</tr>
<tr>
<td>G\textsubscript{1}</td>
<td>160</td>
<td>159 ± 21</td>
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<td>G\textsubscript{3}</td>
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<td>35 ± 9</td>
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<td>G\textsubscript{5}</td>
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<td>4.6 ± 1.2</td>
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<tr>
<td>\zeta\textsubscript{f}</td>
<td>1740</td>
<td>1754 ± 62</td>
</tr>
<tr>
<td>\zeta\textsubscript{d}</td>
<td>1560</td>
<td>1419 ± 151</td>
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<tr>
<td>\Delta (in cm\textsuperscript{-1})</td>
<td></td>
<td>474</td>
</tr>
<tr>
<td>in % of total width</td>
<td></td>
<td>3%</td>
</tr>
</tbody>
</table>

REFERENCE:
NEW TRENDS IN RARE-EARTH ANALYSIS^{1}
N. Spector

Recent analyses of rare-earth spectra were examined and their reciprocal effect on line spectra evaluated. New deductions were made as to the role played by the combination of various light sources, different aspects of the spectra and empirical intensity considerations in the future trends of rare earth analysis.

REFERENCE:
\[ \chi \phi(\bar{r} \to \bar{r}) = \sum_{e} \left[ \int_{\text{forward scattering}} e^{2} \delta(\bar{r}, \frac{1}{2} \bar{r}) \right] \frac{1}{1 - \bar{r}^{2} \bar{r}^{2}} \times \left( \sum_{e' \to e} \Sigma(\bar{r}, e' \to e) \phi(\bar{r}) \right) \]
A GENERALIZED PERTURBATION THEORY AND VARIATIONAL PRINCIPLE FOR MULTIPLE RATIOS OF LINEAR AND BILINEAR FUNCTIONALS

E. Greenspan

Variational principles and a generalized perturbation theory for single ratios of linear or bilinear functionals were recently published by Stacey. The present work extends Stacey's formulation to more general functionals having the form of a product of an arbitrary number of ratios of linear flux functionals and of bilinear functionals. Nuclear systems which are described by the homogeneous or the inhomogeneous Boltzmann equation were considered. The computational strategy and effort required for applying the generalized perturbation theory and variational principle to a multiple ratio were considered and a possible application of the new formulation was described.

REFERENCES:

AN APPROXIMATION TO THE STATIONARY NEUTRON TRANSPORT EQUATION—SIMILAR TO THE Pn APPROXIMATION

M. Lemanska

The neutron flux in slab geometry was obtained in the form
\[ \phi(x,\mu) = f(x) - \mu \frac{df(x)}{dx} + \mu^2 \frac{d^2f(x)}{dx^2} + \ldots + (-1)^{\nu} \mu^\nu \frac{d^{\nu}f(x)}{dx^{\nu}} + \ldots \] (1)
where the function \( f(x) \) is the solution of
\[ f = c \left\{ f + \frac{1}{3} \frac{d^2f}{dx^2} + \frac{1}{5} \frac{d^4f}{dx^4} + \ldots + \frac{1}{2\nu+1} \frac{d^{2\nu+1}f}{dx^{2\nu+1}} + \ldots \right\} \] (2)

Then
\[ f = c \left\{ f + \frac{1}{3} \frac{d^2f}{dx^2} \right\} \] (3)
was used as an approximation to calculate the critical thickness of several assemblies in slab geometry. The results are better than those obtained by the \( P_1 \) approximation as may be seen in Table 1.
**TABLE 1**

**Critical half-thicknesses of an infinite slab**
*(in mean free paths)*

<table>
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<th>c</th>
<th>Exact (1)</th>
<th>P₁ (1)</th>
<th>P₃ (1)</th>
<th>P₅ (1)</th>
<th>Present work</th>
<th>S₂ code</th>
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</thead>
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<td>1.02</td>
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<td>5.663</td>
<td>5.672</td>
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<td>0.530</td>
<td>0.522</td>
<td>0.619</td>
</tr>
</tbody>
</table>

**REFERENCE:**


**EXACT SOLUTION OF THE P₁ TIME-DEPENDENT EQUATIONS WITH TIME-DEPENDENT CROSS SECTIONS FOR SLAB AND SPHERICAL GEOMETRY**

M. Lemanska and Y. Menning*

The P₁ approximation to the time-dependent neutron transport equation with time-dependent cross sections for slab and spherical geometry was solved using the generalized Lie series technique. The variables were separated in the solution obtained, the radial part of which consists of the zero and first spherical moments of the stationary angular flux. In this way the discretization was obtained in the time variable only.

**REFERENCE:**


**ON THE ESTIMATION OF ERRORS IN REACTOR THEORY**

Y. Ronen

A larger scope for the functional analysis method for error estimation was obtained by introducing \( L₁ \) space to the calculations. The advantages of introducing the \( L₁ \) space are the possible close estimation of errors, and a simplification of the calculations. Introduction of the \( L₁ \) space to reactor physics problems also gives some meaning to the interpretation of errors, because this is the natural space for reactor theory problems.

*Swiss Federal Institute for Reactor Research, Würenlingen, Switzerland*
The method was illustrated by some examples dealing with the multi-group diffusion equation, where errors in eigenvalues and in fluxes are estimated and compared with the actual errors.

REFERENCES:
2. Ronen, Y., Nucl. Sci. Eng. 52, 147, (1973)

APPLICATION OF TWO-DIMENSIONAL SPLINE THEORY TO THE SPHERICALLY SYMMETRIC TRANSPORT PROBLEM
L. Finkelstein and A.D. Krumbein

The non-conservation form of the spherically symmetric, energy-dependent transport equation was simulated in a manner which can be solved exactly by a biquadratic spline. The spline was then calculated by a one-step explicit formula. The results obtained thus far, (critical parameters and integrated fluxes), are in excellent agreement with one-speed, one-layer benchmark problems. The cases compared ranged from $c=1.6$, the largest value found in nature, to $c=1.02$, where $c$ is the average number of neutrons emerging from a collision.

The merits of the method are: exact representation of the sources within the framework of splines, simplicity of the numerical algorithm, and reasonably short computing times.

Multistep formulas have been tried for a cubic-quadratic spline and were found to be unstable even for diminishing steps.

REFERENCES:

TWO-DIMENSIONAL NUMERICAL TRANSPORT BY THE METHOD OF CHARACTERISTICS
L. Finkelstein and N. Segev

A little exploited method of solution of the neutron transport equation is to write its leakage term in the form of a full derivative, replace the source term by a sequence of iteratively defined sources, and then solve numerically along the characteristics (straight lines) of the differential operator.

Considerable computational savings which the method provides can be realized
only if
a) a sufficiently simple and accurate cubature formula for the two-dimensional source integral is available, and
b) the numerical solution of the ordinary differential equations along the characteristics can be obtained using relatively large steps.

Our approach to the cubature formula is to divide the surface of the directional sphere into a given number of equally shaped subsurfaces in a way such that a characteristic crosses the centrum of each subsurface. This discretizes the directions of the angular fluxes. Any directional flux is then represented by a one-dimensional spline along its characteristic. This permits large integration steps.

The above method was applied to finite cylinders, infinite cylinders, spheres and slabs. We used one and six energy groups, and also six and eight directions in the cubature formula.

The results were compared with data from benchmarks and also experimentally measured systems. The relative errors in $k_{\text{eff}}$ were of the order of $10^{-2}$ for six directions in the cubature formula, and a fraction of $10^{-3}$ for the eight direction formula. The cases compared ranged from $c=1.6$, the largest value found in nature, to $c=1.02$, where $c$ is the average number of neutrons emerging from a collision.

An additional advantage of the method is algorithmic simplicity, which permits easy programming.

VARIANCE REDUCTION IN DYNAMIC MODELS FOR PARTICLE TRANSPORT SIMULATION

M. Goldstein and B.P. Zeigler

A new formulation of the Monte Carlo method for dynamic models of three dimensional particle transport within a homogenous medium was made \(^{(1)}\). A "basic model" was defined using the standard Monte Carlo procedure. Then two variance reduction techniques, statistical weighting and exponential transform, were formulated in the basic model, so as to produce so-called "biased models". Each biased model was formally shown to produce the same estimate of the parameter of interest (detector response) as the basic model. This was done using methods of comparison of dynamic models derived from system theory. It was also shown that the two variance reduction techniques reduce the running time of the problem significantly.

REFERENCE:


* University of Michigan, Ann Arbor, Michigan, U.S.A.
PARAMETRIC REPRESENTATION OF THE SHIELDING FACTOR CURVES
Y. Gur and S. Yiftah

The self-shielded multigroup cross section set can be divided into two parts: a) infinitely diluted cross sections and scattering matrix elements, which are constants, and b) self-shielding factors (ssf) of two continuous variables (temperature and background cross section). As the ssf are tabulated curves, the user must interpolate between given values and to date there is no single or even accepted solution to the problem of interpolation. Current methods were reviewed\(^{(1)}\) and found to be either complicated or inaccurate (or both).

Parametric representation is a natural means of representing a curve. Two new methods for a parametric representation of the temperature dependent ssf curve were developed\(^{(1)}\), one of which was found to fit the data very well. That representation is obtained as follows. Write:
\[
\log(\sigma_o) = A \text{ arctanh } [m f(\sigma_o) + n] + D
\]
where \(f(\sigma_o)\) is the shielding factor for the background cross section, \(\sigma_o\). Temperature dependence as well as indexes specifying reaction type and group number are omitted. As \(\text{arctanh}(x)\) is defined in the domain \(-1<x<1\) and the shielding factor curve has values in the range \(f(0) \leq f(\sigma_o) \leq 1\), we choose \(m\) and \(n\) so that
\[
m + n = 1 \quad \text{for the upper limit of } f(\sigma_o)
\]
\[
mf(0) + n = -1 \quad \text{for the lower limit of } f(\sigma_o),
\]
by which \(m = 2/[1 - f(0)]\) and \(n = 1 - 2/[1 - f(0)]\).

Denote
\[
C = 1 - f(0)
\]
and obtain
\[
\log(\sigma_o) = A \text{ arctanh } \left[ \frac{2}{C} f(\sigma_o) + 1 - \frac{2}{C} \right] + D.
\]
Any pair of points \([\sigma_o, f(\sigma_o)]\) defines \(A\) and \(D\) which, together with \(C\), completely define the shielding factor curve to be
\[
f(\sigma_o) = 1 - \frac{C}{2} \left[ 1 - \tanh \left( \frac{\log(\sigma_o) - D}{A} \right) \right]
\]
As \(A\), \(C\), and \(D\) are temperature dependent, and \(\log[f(\sigma_o)]\) is linear in \(\log T\), a set of six parameters \([A(T_1), C(T_1), D(T_1), A(T_2), C(T_2)\) and \(D(T_2)]\) completely defines \(f(\sigma_o, T)\).

As different pairs of points belonging to the same curve gave different values for \(A\) and \(D\), a best-fit search in the ranges of \(A\) and \(D\), found by taking
all possible pairs of each curve, was tried and best A and D values to represent the curve were obtained.

More recently, we calculated A and D by each possible pair of points \([\sigma_0, f(\sigma_0)]\). It was found that there always exists at least one pair whose A and D are good parameters for the representation of the entire curve. Moreover, we found that the pair \([10, f(10)]\) and \([100, f(100)]\) yields good representations of the entire set of shielding factor curves of \(^{235}\text{U}\) (better than 2%), \(^{238}\text{U}\) (better than 15% for \(\sigma_0 \leq 100\), and better than 7% in the entire range), \(^{239}\text{Pu}\) (better than 1% for \(\sigma_0 \leq 100\), better than 5% in the entire range), and \(^{241}\text{Pu}\) (better than 1.5% for \(\sigma_0 \leq 100\) and better than 6% in the entire range), while the pair \([100, f(100)]\) and \([1000, f(1000)]\) yields good parametric representation of the entire set of shielding factor curves of \(^{240}\text{Pu}\) (better than 5% for \(\sigma_0 \leq 100\) and better than 20% in the entire range), and of \(^{242}\text{Pu}\) (better than 10% in the entire range). Also, for different temperatures, the deviations of the same \(f(\sigma_0)\) factor were in the same direction and roughly the same percent, which reduces the influence of the deviations on the Doppler coefficient. In the range of importance for fast reactor calculations (above 500 eV), the fit is very good (much better than 1%) for all isotopes, reaction types, temperatures, and background cross sections with the pair \([10, f(10)]\) and \([100, f(100)]\). Thus, instead of calculating many values per curve and representing the shielding factor curve as a table, one can calculate only three values per curve and represent each curve by three parameters per temperature.

A nuclear system representing a large power reactor was calculated with shielding factors obtained from the parametric representation based upon \([10, f(10)]\), and \([100, f(100)]\) and then calculated with exact shielding factors. Very good agreement was found, as may be seen in Table 2.

**TABLE 2**

<table>
<thead>
<tr>
<th>Temp.°K</th>
<th>(k_{\text{eff}})</th>
<th>Doppler coef (\times 10^6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parametric representation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>.92244</td>
<td>.022125</td>
</tr>
<tr>
<td>900</td>
<td>.91512</td>
<td>.010305</td>
</tr>
<tr>
<td>1500</td>
<td>.91223</td>
<td>.004386</td>
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<tr>
<td>Exact</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>.92254</td>
<td>.022239</td>
</tr>
<tr>
<td></td>
<td>.91517</td>
<td>.010358</td>
</tr>
<tr>
<td></td>
<td>.91228</td>
<td>.004383</td>
</tr>
</tbody>
</table>

REFERENCES:
SELF-SHIELDED GROUP CONSTANTS FOR Fast Reactor Calculations

Y. Gur, S. Yiftah, M. Segev and L. Gitter

Two identically generated sets of self-shielded 26-group constants were computed by the code system developed here. The infinitely diluted cross sections and scattering matrix were computed by NANICK(2) and its modified version NAKED(4) from ENDF/B-III(3) tapes and the KEDAK(5) library, respectively. The shielding factors were generated by NASIF(6) from ENDF/B-III tapes and by its modified version NASIFK from the KEDAK file.

The outputs of NANICK and NASIF (ENDF/B-III based data) and of NAKED and NASIFK (KEDAK based data) were combined into two libraries for fast reactor calculations. Elements included in the libraries are H, C, O, Na, Cr, Fe, Ni, 235_U, 238_U, 239_Pu, 240_Pu, 241_Pu and 242_Pu.

Nuclear systems were calculated, and comparative analyses performed(7-10). The differences in the cross sections obtained from different files were studied and a list of cross sections having $k_{eff}$ sensitive to this difference is given in Table 3, in decreasing order of importance.

**Table 3**

<table>
<thead>
<tr>
<th>Sensitivity list for $k_{eff}$ in order of importance</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Pu-239 fission cross section in the range 1 to 100 keV</td>
</tr>
<tr>
<td>2. U-238 capture cross section in the range 1 to 1000 keV</td>
</tr>
<tr>
<td>3. Pu-239 capture cross section in the range 1 to 100 keV</td>
</tr>
<tr>
<td>4. U-238 inelastic cross section in the range 10 to 1000 keV</td>
</tr>
<tr>
<td>5. U-235 fission cross section in the range 50 to 1000 keV</td>
</tr>
<tr>
<td>6. U-238 elastic cross section in the range 10 to 10,000 keV</td>
</tr>
<tr>
<td>7. Pu-239 ν in the range 1 to 3000 keV</td>
</tr>
<tr>
<td>8. Fe ν in the range 10 to 10,000 keV</td>
</tr>
</tbody>
</table>

A comparison between plutonium and uranium cross sections is given in Table 4.

REFERENCES:
2. Gur, Y., TNSD-R/419, Appendix No. 5.
### Table 4
Pu and U cross sections from ENDF/B-III and KEDAK

<table>
<thead>
<tr>
<th>Group</th>
<th>Lower energy (eV)</th>
<th>Upper energy (eV)</th>
<th>Uranium-235 fiss</th>
<th>Uranium-238 capture</th>
<th>Plutonium-239 fission</th>
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<tbody>
<tr>
<td></td>
<td>ENDF/B-III</td>
<td>KEDAK</td>
<td>ENDF/B-III</td>
<td>KEDAK</td>
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<td>1</td>
<td>6.500E+06</td>
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<tr>
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<td>4.000E+06</td>
<td>6.500E+06</td>
<td>1.074E+00</td>
<td>1.187E+00</td>
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<td>10</td>
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<td>1.541E+02</td>
<td>7.834E-01</td>
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</table>
PRACTICAL PREPROCESSED NUCLEAR DATA FILES FOR FAST REACTOR CALCULATIONS
Y. Gur and S. Yiftah

Basic nuclear data libraries, such as ENDF/B-III, are used today for the generation of multigroup cross section sets. Since the multigroup sets are determined by calculating the weighted averages of the cross section curves, knowledge of the weighting function within each group is required. In principle, this function is not only dependent on the specific reactor, but is also a function of position in the reactor. With existing codes and methods the weighing function in the Bondarenko type library is not iterated, since each time the weighing function is changed, a code that handles the basic data library and consumes much computer time must be run.

A new method that enables the user to obtain effective, self-shielded multigroup cross section sets averaged over any desired weighting function in a few computer seconds from a preprocessed library, without reference to the basic data library, was developed (1). The preprocessed library is only 2-3 times as large as a Bondarenko type library and may be generated using existing codes.

A family of functions with terms into which any weighting function can be expanded is used. Group averages of each cross section with respect to terms of the family and a set of shielding factors form the preprocessed library. Two families of functions, $f_n(E)$, are considered, and two methods are given for the expansion of $W(E)$ into each series of $f_n(E)$. Nuclear parameters obtained via these methods were compared with the same parameters obtained using the exact weighting function (SNEAK flux) to check the methods. Very good agreement was found.

A preprocessed compact library of ENDF/B-III materials is available, upon request, from the authors.

REFERENCES:
1. Gur, Y., and Yiftah, S., IA-1293, 1974

COMPARATIVE ANALYSIS OF AMERICAN AND GERMAN NUCLEAR DATA FILES FOR THE CALCULATION OF FAST FISSION REACTORS
S. Yiftah, Y. Gur, M. Segev and L. Gitter

The main sources of nuclear data for fast reactor calculations are the American ENDF/B-III, the German KEDAK, the British UKNDL and the Russian evaluated nuclear data files. Every country uses its own evaluated files and code package to obtain the physics parameters of the designed reactors and the question being
asked is whether these physics parameters would remain the same had another source been used as an input for the calculation.

A code package named NANICK, which handles both ENDF/B-III and KEDAK via the same algorithm generating multigroup-self-shielded neutron cross section sets and calculates physics parameters of nuclear systems, was completed and used to calculate a number of fast nuclear systems and critical experiments in a spherical approximation. These calculations are used as a tool for detecting discrepancies between nuclear data from different files.

It was shown\(^{(1-3)}\) that ENDF/B-III and KEDAK predict different physics parameters for fast reactors. A perturbation analysis of these discrepancies has led to the identification of significant differences between KEDAK and ENDF/B-III cross sections. These differences are mainly in the fission and capture cross sections of Pu-239, in the capture and inelastic cross sections of U-238, and in the huge Na resonance. Viewing file differences as the reflection of the experimental state of the art, and based on a goal of 1\% accuracy in \(k_{\text{eff}}\) prediction, the needed accuracy in cross section measurements was determined.

REFERENCES:

EVALUATION OF NUCLEAR DATA FOR ACTINIDE ISOTOPES
M. Caner and S. Yiftah

A survey was made of isotopes from U to Cm for which a new nuclear data evaluation might be of interest. The factors affecting the choice of a given isotope were:

a. which isotopes influence fast breeder reactor economics\(^{(1-3)}\).
b. which evaluations are available\(^{(4,5)}\), and which isotopes are included in the ENDF/B and UKNDL files\(^{(5)}\).
c. which experimental data are available\(^{(4-13)}\). Here we were interested in seeing if there were more recent data than those in the last available evaluation, and if there was enough information to perform optical model and statistical theory calculations.
d. for which isotopes were requests for new nuclear data measurements made by reactor physicists. Here, in particular, we examined the new experimental data to see if they satisfied the requests.

In the light of the above considerations an evaluation of the isotopes $^{238}\text{Pu}$, $^{241}\text{Am}$, and $^{244}\text{Cm}$ was begun.

$^{238}\text{Pu}$ is an alpha-emitter and is important as a heat source; it has found application in power supplies in space and in heart pacemakers. $^{241}\text{Am}$ has potential uses as a heat source (through alpha-ray emission), as a gamma-ray source and as a target for $^{242}\text{Cm}$. $^{244}\text{Cm}$ is used as a target material for the production of $^{252}\text{Cf}$ and as a heat source. The above mentioned isotopes are economically significant, since they reduce the price of reprocessed nuclear fuel.

REFERENCES:

10. Ellis, Y.A., Nuclear Data Sheets B6, 257 (1971)
12. Ellis, Y.A., Nuclear Data Sheets B6, 539, 621 (1971)

A NEW EVALUATION OF NUCLEAR DATA FOR PLUTONIUM-240, 241, 242(1)

M. Caner, S. Yiftah, B. Shatz* and R. Meyer*

The isotopic composition of the plutonium produced as a by-product in thermal reactors, which is to serve as fuel for fast reactors, may be typically in the following range: Pu-239, 50-65%; Pu-240, 20-25%; Pu-241, 10-15%; Pu-242, 5-10%. This means that for a typical 1000 MWe fast reactor fueled with about three tons of plutonium, almost half, or 1.5 tons, may consist of higher plutonium isotopes. This emphasizes the importance of having data files which reflect the latest available experimental information and evaluated data for these isotopes. Current data files for Pu-240, Pu-241 and Pu-242 are based on data prior to the following dates: KEDAK, 1967; ENDF/B-III, 1968 for Pu-240, 1970 for Pu-241, 1967 (with resonances revised in 1971) for Pu-242.

* Kernforschungszentrum, Karlsruhe, Federal Republic of Germany
New experimental data are available on resonance parameters and fission cross sections. In addition, there are new measurements of the total and scattering cross sections of Pu-240 in the keV range.

A new evaluation of nuclear data for Pu-240, Pu-241 and Pu-242, based on the new experimental information and nuclear model calculations, has been performed by us\(^{(2-4)}\). The numerical data have been incorporated into the new KEDAK file.

In the present work we have reviewed the most significant nuclear data for Pu-240, 241, 242 and compared them with the ENDF/B-III file and with our previous 1967 evaluation forming part of the KEDAK file. Discrepant data and parts of the evaluations based on nuclear model calculations are emphasized.

REFERENCES:
2. Caner, M., and Yiftah, S., IA-1243 (1972)
3. Caner, M., and Yiftah, S., IA-1276 (1973)

NASIF: CODES FOR COMPUTING GROUP SHIELDING FACTORS FROM RESONANCE PARAMETERS
Y. Gur and S. Yiftah

Four versions of NASIF, computer codes for calculating group shielding factors from resonance parameters, have been completed.

Version 1 is a fully automatic code for computation from ENDF/B-III tapes\(^{(1)}\). This version treats an entire ENDF/B-III tape in one run. It is automatic in the sense that the user is not required to be familiar with the contents of the basic data library. Only the identifying numbers of the isotopes whose shielding factors are to be computed are needed. In this version the integration of the cross section is performed with only three resonances (i.e. the resonance nearest the energy point and one resonance on each side of it) contributing to the computed cross section.

Version 2 differs from version 1 in that the number of "side" resonances is specified by the user (as input data, up to 12 "side" resonances from each side are permitted). If one "side" resonance is requested the results are identical to those of version 1.

Version 3 differs from version 2 in that the central and one "side" resonance contribute to the calculated cross section in the integration, while the contribution of the wings of 11 "side" resonances from each side is collapsed...
into a parabola. This version yields results identical to those of version 2 with 12 "side" resonances, yet is as quick as version 1 in computing group shielding factors.(2)

Version 4 computes shielding factors from KEDAK resonance parameters.

Versions 2, 3 and 4 read basic data from cards either punched from ENDF/B-III tapes or prepared from KEDAK data in the ENDF/B-III format.

Table 5 shows result obtained by the three ENDF/B-III versions.

<table>
<thead>
<tr>
<th>Group</th>
<th>Energy range (eV)</th>
<th>Number of side resonances (Version 2)</th>
<th>Version 3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>1</td>
<td>100-215</td>
<td>0.367</td>
<td>0.380</td>
</tr>
<tr>
<td>2</td>
<td>46.5-100</td>
<td>0.232</td>
<td>0.243</td>
</tr>
<tr>
<td>Time on IBM/370 (sec)</td>
<td>10</td>
<td>13</td>
<td>16.5</td>
</tr>
</tbody>
</table>

REFERENCES:

THE HASHOV CODE
A.D. Krumbein

A program, HASHOV, was written in FORTRAN IV for use on the 370/165 IBM computer. It combines the Hansen exponential transformation method(1) for the solution of the space-time dependent diffusion equation in one space dimension, with certain advantageous features of the SHOVAV(2) code. These include the capability of calculating cross section mixing and shielding factors, temperature feedback and several forms of reactivity insertion. Steady-state xenon and xenon feedback routines have also been included.

The code has been successfully checked against the results of prompt excursion problems originally analyzed by Yasinsky and Henry(3).

REFERENCES:
2. Saphier, D. and Yiftah, S., IA-1217 (1971)
LASER-INDUCED PLASMA RESEARCH
LATTICE DYNAMICAL ANALYSIS OF THE MöSSBAUER EFFECT OF $^{57}$Fe IN NATURAL IRON

R. Ruppin

A quasiharmonic, pressure dependent, lattice dynamical model was employed in order to calculate the recoilless fraction and the second order Doppler shift of $^{57}$Fe in natural iron. From a comparison of the calculated and the experimental temperature dependence of the recoilless fraction it was concluded that the dominant anharmonic contribution to this quantity arises from cubic anharmonicity. The pressure dependence of both the recoilless fraction and the second order Doppler shift, as calculated from the lattice dynamical model, agrees with that predicted by the Debye model.

REFERENCE:

HYPERFINE INTERACTIONS AND RELAXATION EFFECTS IN LAVES-PHASE INTERMETALLIC COMPOUNDS OF NEPTUNIUM


Studies of magnetic properties of cubic Laves-phase compounds of Np were performed using the Mössbauer effect of the 59.5 keV transition in $^{237}$Np. The compounds studied were NpAl$_2$, NpCo$_2$, NpNi$_2$, NpFe$_2$, and NpIr$_2$. Hyperfine-interaction parameters and ordering temperatures were deduced from these measurements. If the values of $H(T)/H(0)$ are plotted as a function of $T/T_c$, the points (except those of NpFe$_2$) lie on the molecular-field-theory curve for $S=1/2$. Quadrupole interactions were found to be very small. This behavior is consistent with the assumption that the ground crystalline state in these compounds is an isolated Kramers doublet. Relaxation phenomena were observed in the spectra. The spectra could be fitted by assuming relaxation effects within the Kramers doublet with a relaxation time of $\approx 4 \times 10^{-11}$ sec. Isomer shifts were measured and found to change regularly with the size of the unit cell.

REFERENCE:

*Hebrew University, Jerusalem
SPIN-ORIENTATION DIAGRAMS AND MAGNETIC ANISOTROPY OF RARE-EARTH IRON TERNARY CUBIC LAVES COMPOUNDS\(^{(1)}\)

U. Atzmony, M.P. Dariel, E.R. Bauminger\(^{*}\), D. Lebenbaum\(^{*}\), I. Nowik\(^{*}\), and S. Ofer\(^{*}\)

The directions of the easy magnetization in the \(\text{Ho}_{x} \text{Tb}_{1-x} \text{Fe}_2\), \(\text{Ho}_{x} \text{Er}_{1-x} \text{Fe}_2\), \(\text{Dy}_{x} \text{Tb}_{1-x} \text{Fe}_2\), \(\text{Dy}_{x} \text{Er}_{1-x} \text{Fe}_2\), and \(\text{Ho}_{x} \text{Tm}_{1-x} \text{Fe}_2\) systems were determined as a function of \(x\) and temperature by means of the Mössbauer effect in \(^{57}\text{Fe}\). If the direction of magnetization of each system is described by an \((x,T)\) spin-orientation diagram, it is found that the \((x,T)\) plane is divided into two or three regions, in each of which the direction of magnetization is along a different major crystal axis. Theoretical calculations based on the assumption that the magnetic crystalline anisotropy is due to the anisotropy of the interaction between the \(4f\) electrons of the rare-earth ions with the crystal fields reproduced the general features of the experimental results though small discrepancies remained. Taking into account an additional contribution to the anisotropy attributed to the Fe-Fe interaction improved the agreement between the theoretical and experimental spin-orientation diagrams. From the theoretical fits to the experimental results a value of \((-0.38\pm0.003)a_0^{-2}\) was derived for the ratio of the crystal field parameters \(A_6/A_4\). The transitions between the regions of the spin-orientation diagrams are not sharp. Possible reasons for the existence of the transition regions were considered.

REFERENCE:

MAGNETIC HYPERFINE INTERACTION IN KFeCl\(_3\): A COMPOUND WITH ONE-DIMENSIONAL SPIN CORRELATIONS

E. Gurewitz, J. Makovsky and U. Atzmony

The present work is a Mössbauer effect (M.E.) study on the 14.4 keV transition of \(^{57}\text{Fe}\) in KFeCl\(_3\). Recent neutron diffraction studies\(^{(1)}\) indicate that the compound is paramagnetic at room temperature and undergoes a transition at \(T_N = 16\) °K, to an antiferromagnetically ordered state. This state consists of ferromagnetic chains coupled antiferromagnetically to each other. The spin directions are parallel to the chain axis. The intrachain ferromagnetic interactions are much stronger than the interchain antiferromagnetic interactions, causing one-dimensional magnetic correlations in the temperature range \(T_N < T < 2T_N\).

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Measurements at some of the temperatures in the range $T_N < T < 2T_N$ showed a distinct hyperfine magnetic splitting. This splitting is due to one-dimensional magnetic correlations and, to the best of our knowledge, are shown and analyzed in this work for the first time\(^{(2)}\). The spectra exhibit a typical relaxation character which is caused by an alternating effective hyperfine field. The "flips" of this field from $+H_{\text{eff}}$ to $-H_{\text{eff}}$ and vice versa are due to one-dimensional spin correlations and magneto-crystalline anisotropy interaction.

REFERENCES:

DIPOLAR CONTRIBUTIONS TO MAGNETIC HYPERFINE FIELDS IN $\text{Er}_x\text{Y}_{1-x}\text{Fe}_2$ AND $\text{Tb}_x\text{Y}_{1-x}\text{Fe}_2$ COMPOUNDS\(^{(1)}\)

M.P. Dariel, U. Atzmony and D. Lebenbaum

Mössbauer effect measurements on $^{57}\text{Fe}$ were carried out in the pseudo-binary systems $\text{Er}_x\text{Y}_{1-x}\text{Fe}_2$ and $\text{Tb}_x\text{Y}_{1-x}\text{Fe}_2$ at $4.2^\circ$, $80^\circ$, and $300^\circ$K. The isotropic part of the hyperfine field acting on the iron nuclei includes a term due to polarization by the localized rare-earth spin. Magnetic dipolar contributions account only in part for the differences in the magnitude of the hyperfine fields at the inequivalent sites.

REFERENCE:

$^{119}\text{Sn}$ NGR STUDY OF MOLECULES ADSORBED ON GRAPHITE\(^{(1)}\)

S. Bukhpahan, T. Sonninu, and J.G. Dash

The Mössbauer effect in $^{119}\text{Sn}$ was employed to study the physical adsorption properties of molecules of $\text{Sn(CH}_3)_4$, $\text{SnCl}_4$, and $\text{SnI}_4$ adsorbed on graphite.

The recoilless fraction $f$ was measured as a function of temperature in the range $70^\circ$-$200^\circ$K, (Fig. 1), and a characteristic Debye temperature was obtained. To calculate the binding energy of these molecules to graphite

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a single Lennard-Jones potential was assumed as a function of the separation distance between the molecules and the substrate. This energy was computed to be 10, 11.8 and 73 kcal/mole for Sn(CH₃)₄, SnCl₄, and SnI₄, respectively.

REFERENCE:

MOLECULAR COMPLEXES OF I₂ - A MOSSBAUER EFFECT STUDY(1)
S. Bukshpan, C. Goldstein, T. Sonnino, L. May* and M. Pasternak

Molecular complexes of I₂ with different organic solvents, in frozen solutions, were studied using the Mössbauer effect in ¹²⁹I. The results obtained for the hyperfine constants indicated that the complexes may be divided into three main groups with increasing bond strength, according to the organic solvent used: a) π solvents, b) alcohols and ether, and c) amines. The same classification was also used in the analysis of various

*Tel Aviv University, Ramat Aviv
Permanent address: Catholic University of America, Washington, D.C.
properties of the I_ complexes. Some general conclusions on the electronic
nature of the I_-complexant bond were derived.

REFERENCE:
1. Bukshpan, S., Goldstein, C., Sonnino, T., Hay, L. and Pasternak, M.,

MAGNETIC STRUCTURE DETERMINATION OF NiI_2 BY THE 129 I NÖSSBAUER EFFECT(1)
M. Pasternak, S. Bukshpan and T. Sonnino

The spin arrangement in antiferromagnetic NiI_2 (T_N = 75^0 K) was deter-
dined by the Mössbauer effect (ME) in 129 I.

Above the transition temperature T_N the ME spectrum indicates a quadrupole
interaction that for symmetry reasons has the principal axis of the electric
field gradient (egf) in the direction of the [111] crystal axis. Below the
T_N the Mössbauer spectrum is characteristic of combined quadrupole and magnetic
dipole interaction with an angle θ between the principal axis of the efg and
the magnetic field of 55^0. This suggests a collinear spin arrangement with
moments alternating in direction among the various (100) planes.

REFERENCE:

14 N PNQR INVESTIGATION OF THE EFFECT OF PRESSURE ON THE PHASE TRANSITION IN
MALONONITRILE
A. Zussman and E. Rapoport

The 14 N pure nuclear quadrupole resonance frequencies of malononitrile
were measured as a function of pressure up to 6 kbar at constant temperature
(24°C). The second order phase transition, previously studied by Zussman and
Alexander(1), was observed at P_C = 200 bar and 24°C.

Below P_C, 4 lines, belonging to two nonequivalent nitrogen nuclei, are
observed. Above P_C each line splits into two lines indicating a change in the
symmetry of the crystal. This splitting Δν is proportional to the order
parameter of the transition and therefore, near P_C, is expected to obey the
relationship

Δν ∝ (P - P_C)^α

where α is the critical exponent. α was found to be close to 1/2 and is in
accord with Landau's theory. A maximum splitting of about 50 kHz at 6 kbar
was found. A more detailed study is in progress.
EFFECT OF PRESSURE ON $^{14}$N NUCLEAR QUADRUPOLE RELAXATION IN HEXAMETHYLENETETRAMINE$^1$

A. Zussman and E. Rapoport

$^{14}$N nuclear quadrupole resonance frequencies and spin-lattice relaxation time, $T_1$, in hexamethylenetetramine (HMT) were measured as a function of hydrostatic pressure up to 6 kbar at 257°, 273°, 294.5°, 309°, and 317°K. For the three higher isotherms $T_1$ depends exponentially on pressure up to 3 kbar. In this region $T_1$ is determined mainly by molecular reorientation of the tetrahedral HMT molecule around its four 3-fold axes. This mechanism was considered in terms of a simple activation process. The activation volume, $\Delta V^* = 23.6 \pm 1 \text{ cm}^3/\text{mole}$, and activation enthalpy, $\Delta H^* = 17 \pm 1 \text{ kcal/mole}$ were determined. From thermal expansion and compressibility data, a thermal pressure, $p_T = T(\partial p/\partial T)_V$, of 6.2 kbar and an activation energy $E^*$ of 12 to 15 kcal/mole were deduced. These values of $\Delta H^*$, $\Delta E^*$ and $\Delta V^*$ are higher than the corresponding values reported by Anderson and Slichter$^2$ for three other organic solids and might indicate the effect of the large number of hydrogen bonds in HMT.

REFERENCES:

NMR STUDY OF NON-STOICHIOMETRIC TiD$_x$

Drora Kedem and D. Zamir

TiD$_x$ is a defect structure system, i.e., for $x<2$ there are vacancies in the deuterium cubic sublattice. Each vacancy produces an electric field gradient causing the neighboring deuterium atoms to experience a quadrupole interaction. One way to measure this interaction is to measure the NMR absorption line width and intensity.

Several samples of TiD$_x$, with values of the atomic ratio $x$ varying up to a maximum of 2, were investigated using a Varian CW spectrometer. The resulting absorption line derivatives were integrated twice, thus yielding the relative integrated intensities of the NMR lines.

Figure 2 is a plot of the relative intensity S vs. the atomic ratio $x$. The line intensity decreases faster than $x$, as if part of the deuterium nuclei
are not contributing to the NMR line when $x$ decreases. Since when $x$ decreases the cubic symmetry of the deuterium sub-lattice is disturbed, those deuterium atoms which are near the vacancies will experience a quadrupole interaction large enough to delete their contribution to the resonance line. The (a) line in Fig. 2 gives the probability for a deuterium atom in the TiD$_x$ sample to have a missing nearest neighbor. It can be seen that the decrease in the line intensity using this model is too steep. The line (b) gives the probability for a deuterium atom to have two or more missing neighbors, which will cause a quadrupole interaction about twice as large as in the case of only one missing neighbor. The "knee" for $x$=1.6 is based on the phase diagram of the TiD$_x$ system. This model explains the decrease in the line intensity, as well as an increase in the line width for $x$<2, caused by the quadrupole interaction experienced by those deuterium atoms having only one missing nearest neighbor.

One can calculate the quadrupole interaction caused by a single vacancy, assuming a point charge model

$$eq = e^{-kr}(1 + kr + \frac{(kr)^2}{2}) \cdot \frac{(3z^2 - r^2)e}{r^5}$$

Using the experimental value of $eq$ we can obtain information about $k$, the screening factor.
Spin lattice relaxation time of $^{109}$Ag in silver metal was measured in the solid and liquid states, from room temperature to $1085^\circ$C. The measurements were performed at a frequency of about 12 MHz in a magnetic field of about 60 kOe, produced by a superconducting magnet and a single coil phase coherent NMR system.

In continuation of the above studies, spin-spin relaxation time was measured from room temperature to $670^\circ$C, in a field of 22 kOe produced by an electromagnet. S/N problems in $T_2$ measurements, resulting from working in a relatively low field, limited the temperature range in this case.

The measured $T_2$ in silver results from the spin-dipolar interaction and the spin-lattice relaxation time. As a result of the small magnetic moment of silver, $T_2$ is relatively longer than in other solids and $T_1$ is of the same order of magnitude as $T_2$. Moreover, with increasing temperature, $T_2$ becomes equal to $T_1$ even before the onset of motional narrowing. This special behavior of silver is demonstrated in Fig. 3. Also shown is Narath's

![Graph](image-url)
result for $T_2$. We derived the spin-dipolar relaxation time $(T_2)_d.d$ from $T_1$ and $T_2$ data. The figure shows $(T_2)_d.d$ behavior and the onset of motional narrowing.

REFERENCES:

EXPERIMENTAL AND THEORETICAL STUDIES OF DEFECTS IN HEXAGONAL BORON NITRIDE
A. Katzir, J.T. Suss, A. Zunger and A. Halperin

Measurements of electron paramagnetic resonance (EPR), thermoluminescence and thermally stimulated current were performed on hexagonal boron nitride (HBN). A model was proposed to explain these results. It is suggested that carbon impurities introduce luminescence centers with energy levels at $(4.1\pm0.1)$ eV below the conduction band. Ionizing radiation frees electrons from the levels; some of these electrons may fall back and emit blue luminescence. Others may be trapped either in nitrogen vacancies (three-boron-centers) or in one-boron-centers at, respectively, $(1.0\pm0.1)$ eV and $(0.7\pm0.1)$ eV below the conduction band. When the samples are heated, the electrons escape from the traps resulting in a decrease in the EPR signal and the appearance of glow curves.

We have shown by quantum mechanical point defect molecular cluster calculations that in HBN:

a) An electron can be trapped in a nitrogen vacancy at about $1.0$ eV below the conduction band. The charge distribution at this defect level suggests a three-boron-center character.
b) Carbon impurities should introduce an energy level at about $4.0$ eV below the conduction band.

The calculations thus support the proposed model.

REFERENCE:

POINT DEFECTS IN HEXAGONAL BORON NITRIDE: THEORETICAL STUDIES
A. Zunger and A. Katzir

Substitutional and displaced carbon impurities and an isolated nitrogen vacancy in hexagonal boron nitride were theoretically investigated by the 'small periodic cluster' approach. The perfect solid band structure was

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calculated from the solution of the eigenvalues of a finite and periodic cluster of atoms arranged according to the known crystal structure. The linear combination of atomic orbitals (LCAO) representation of the crystal orbitals was adopted and semiempirical molecular orbital (MO) methods (Extended Huckel, Iterative Extended Huckel) were used for the solution of the electronic eigenvalue problem. Point defect problems were then treated by introducing the impurity atom or the vacant site into the otherwise perfect periodic cluster, and repeating the solution. Lattice relaxations were introduced around the defect site and charge redistribution among the cluster atoms was allowed for via self-consistent MO treatment.

For a substitutional carbon impurity defect, it is observed that two deep defect levels, mainly localized on the carbon atom, appear (3.2-4.9 eV below the conduction band). Another level splits from the conduction band as the carbon atom is raised from the layer plane in a perpendicular direction. This level, 1.0-1.3 eV below the conduction band, has a symmetrical charge distribution on the three boron atoms surrounding the impurity site. As the distance of the carbon atom from the layer plane is increased to infinity, a nitrogen vacancy is formed. It is characterized by a defect level 1.1-1.4 eV apart from the conduction band edge which also possesses a three-boron character. Lattice relaxations were shown to stabilize these defects. The findings agree semiquantitatively with the experimental results on these defects.

REFERENCE:

EPR OF Gd IN SINGLE CRYSTALS OF Pd

The fine structure of Gd ions in single crystals of Pd was investigated experimentally for low Gd concentrations (200-500 ppm), at helium temperatures and at 9.4 Gc/sec. The results show that the spectrum is strongly temperature dependent. Very good agreement was obtained between the experimental and theoretically predicted results. The range of interaction between the Gd ions

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was found to be about six lattice constants. This value was derived from the intensity of an additional resonance line, as a function of concentration, that was assumed to be due to resonance on non-isolated Gd ions.

**DYNAMIC JAHN-TELLER EFFECT IN THE EPR SPECTRUM OF Ni**

A. Schoenberg, J.T. Suss, Z. Luz* and W. Low**

An electron spin resonance study of the dynamic Jahn-Teller effect in Ni**1+** and Ni**3+** in MgO at liquid helium temperature was carried out. For both ions the spectra arise from strain split ground vibronic doublets, with a small admixture of an excited singlet. From the anisotropy of the line-width it follows that the symmetry of this singlet is A2 for Ni**1+**, and A1 for Ni**3+**.

REFERENCE:

**EPR STUDY OF Ru**

A. Raizman and J.T. Suss

The EPR spectra of arc grown single crystals of CaO doped with Ru and Rh were studied. The spectrum of Ru ions was observed at 4.2°K and is attributed to Ru**3+** with a 2T2g(4d5) ground state in a strong octahedral crystal field. The spectrum can be described by an isotropic spin hamiltonian: \( \mathcal{H} = g \beta H . S + A I . S \) with \( S = 1/2 \), \( ^{99}I = 5/2 \) and \( ^{101}I = 5/2 \). The parameters of the spin hamiltonian are: \( g = 1.8307 \pm 0.0002 \); \( ^{99}A = (52.0 \pm 1.0)G \) and \( ^{101}A = (58.5 \pm 1.0)G \). These values are close to those reported for Ru**3+** in MgO**2**.

The spectrum of Rh ions consists of a single isotropic line at 93°K and of an anisotropic, tetragonal spectrum, characteristic of three ions per unit cell, between 1.5° - 4.2°K. At 93°K the isotropic line has a \( g = 2.287 \pm 0.001 \) and a 9G peak-to-peak linewidth of the first derivative of the absorption line with \( H_{dc} \) along the [111] direction, which does not permit resolution of the hyperfine structure. The low temperature spectrum

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can be fitted to an axial spin hamiltonian \( \mathcal{H} = g_{\parallel} H S_z + g_{\perp} B (H S_x + H S_y) + A \downarrow S_z A \downarrow (I S_x + I S_y) \) with \( S = 1/2 \), \( I = 1/2 \), \( g_{\parallel} = 2.0392 \pm 0.0003 \), \( g_{\perp} = 2.4053 \pm 0.0003 \), \( A \downarrow = (3.8 \pm 0.2) G \) and \( A_{\parallel} < A_{\perp} \) (not resolved). The spectrum of Rh is characteristic of a static Jahn-Teller effect. This spectrum can be either due to Rh\(^{2+}(4d^7)\) or Rh\(^{2+}(4d^9)\) both having the same \( ^2E_g \) ground state in a strong octahedral crystal field.

REFERENCES:

DIFFUSION OF \(^{140}\)La IN bcc \(\gamma\)-LANTHANUM AND \(\delta\)-CERIUM\(^{1}\)

M.P. Dariel

The serial-sectioning method was used to determine the self-diffusion coefficients in bcc \(\gamma\)-lanthanum and the solute diffusivities of lanthanum in bcc \(\delta\)-cerium. The results are given by

\[ D_{\text{La}}^{\text{La}} = 1.3 \times 10^{-2} \exp(-24500/RT) \text{ cm}^2/\text{sec} \]

and

\[ D_{\text{La}}^{\text{Ce}} = 3.8 \times 10^{-2} \exp(-24500/RT) \text{ cm}^2/\text{sec} \]

The similarity of the diffusion characteristics in the different rare-earth metals casts doubt on the validity of the activated interstitial model put forward in order to account for the peculiar diffusion behavior in the bcc phases of cerium and plutonium.

REFERENCE:
1. Dariel, M.P., Phil. Mag. 28, 915 (1973)

Co DIFFUSION IN VANADIUM SINGLE CRYSTALS

J. Pelleg

Diffusion of \(^{60}\)Co in vanadium single crystals is being investigated over a wide range of temperatures (800° - 1800°C) by applying special micro-sectioning\(^{(1)}\), grinding and lathe sectioning techniques. Preliminary results indicate that diffusion of Co in vanadium is faster by about one order of magnitude than the self-diffusion of vanadium\(^{(2)}\).
The data in the temperature range 1000°-1490°C fit the equation

\[ D = 0.47 \exp\left(-67960/RT\right). \]

REFERENCES:

SELF-DIFFUSION IN VANADIUM SINGLE CRYSTALS \(^1\)

J. Pelleg

Self-diffusion of \(^{48}\text{V}\) in vanadium single crystals was reinvestigated over the temperature range 724°-1642°C. Contributions to diffusion from migration along short-circuit paths at the lower temperatures was avoided by applying a microsectioning technique specially developed for this study. The change in slope of the Arrhenius curve reported to occur at about 1350°C was not observed in this investigation, however it was observed in the vicinity of 1642°C. The data in the temperature range 724°-1642°C can be fitted to the relation

\[ D = (2.88^{+0.4}_{-0.3}) \times 10^{-1} \exp\left[-(73936\pm306)/RT\right], \]

consistent with normal diffusion by a single-vacancy mechanism. Above 1642°C the data fit the equation

\[ D = (1.73^{+0.99}_{-0.63}) \times 10^2 \exp\left[-(97753\pm1816)/RT\right]. \]

REFERENCE:

NEUTRON DIFFRACTION STUDY OF CsMn\(_4\)Cl\(_9\)

E. Gurewitz, J. Makovsky and H. Shaked

The structure of CsMn\(_4\)Cl\(_9\) belongs to the tetragonal space group \(\text{C}_{4h}^{2+} \text{I}_{4}^{1}/a\) with lattice constants: \(a = 11.68\), \(c = 10.36\) \(\text{Å}\) \(^1\). The Mn\(_{2+}\) ions are located at the centers of \(\text{Cl}^-\) octahedrons. Single crystals of CsMn\(_4\)Cl\(_9\) were grown from non-stoichiometric melts, and ground into polycrystalline samples. A neutron diffraction study of these samples revealed that the compound undergoes a transition to antiferromagnetism at \(T_N = 17\)°K. Analysis of its crystallographic and magnetic structures is underway.

REFERENCE:
A NEUTRON DIFFRACTION STUDY OF MAGNETIC STRUCTURES AND MAGNETIC INTERACTIONS IN ORTHOCROMITES

N. Shamir, H. Shaked and S. Shtrikman*

The magnetic structures of most of the orthochromites (RCrO$_3$, where R is a rare-earth element or Y) which were reported in the literature were derived from neutron diffraction of powder samples (1,2). Some of these structures (R=Ho, Er, Yb, Tm, Lu) were reported to be nonaxial with fixed spin orientation relative to the crystallographic axes over a wide range of temperatures (1). This is in disagreement with results of macroscopic magnetic measurements (3).

In order to resolve this discrepancy we obtained long wavelength ($\lambda \approx 2.4 \AA$) neutron diffraction patterns of powder samples of orthochromites. A preliminary analysis of samples with R=Ho, Er, Yb, Tm leads to axial spin structures in agreement with the macroscopic measurements (3). Intensity-temperature curves were obtained for R=Y, La, Nd, Dy, Ho, Er, Yb, Lu. These curves lead to a Brillouin-like behavior. Spin reorientation was observed in the case of ErCrO$_3$. In HoCrO$_3$, no reorientation was observed in disagreement with other reports (1). With TbCrO$_3$, superlattice lines were observed at 1.5K. Investigations of some single crystals are presently underway in order to find out whether or not the canting angle of the spins depends on the temperature, and to see possible spin reorientations that can not be seen from powder samples.

REFERENCES:

SEARCH FOR THE OPTIMAL SET OF MONOCHROMATOR AND COLLIMATORS IN A NEUTRON DIFFRACTION SPECTROMETER

H. Pinto and H. Shaked

In powder analysis by neutron diffraction three important factors are taken into consideration: a) resolution, b) counting statistics (intensity) and c) time needed to perform the experiment. A good indicator of the resolution is the full width at half maximum (FWHM). The FWHM, is a function

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of the angular divergence of the collimators, the mosaic spread of the monochromator, and a resolution parameter \( a \) \(^{(1,2)} \) (\( a = \tan \theta_s / \tan \theta_m \) where \( \theta_s \) and \( \theta_m \) are the Bragg angles of the sample and the monochromator, respectively). Unfortunately, the counting rate is competitive with these parameters. As it is therefore of interest to have an idea of the performance to be expected from the various sets of collimators and monochromators available in our laboratory, a series of measurements with the U.S. 1 diffractometer at the IRR-2 is underway.

The powder sample chosen for this investigation was \( Y_2O_3 \) and monochromators of pyrolytic graphite, copper and aluminium are being investigated. Where good resolution is required, it is advantageous to use long wavelength neutrons and preliminary results indicate that if pyrolytic graphite is used as a monochromator, good resolution is obtained with no significant decrease in intensity.

REFERENCES:


NEUTRON DIFFRACTION STUDY OF THE SPIN REORIENTATION IN \( Ho_{0.6}Ta_{0.4}Fe_2 \)
G. Dublon, M.P. Dariel, U. Atzmony and H. Shaked

Mössbauer effect studies have revealed the presence of several spin reorientations in ternary cubic rare-earth iron Laves compounds. The single ion model, which has been successfully used to account for the magnetic anisotropic behavior of these compounds, predicts the spin reorientation to be a first order type transition. Mössbauer effect\(^{(1)}\), elastic data\(^{(2)}\) and specific heat\(^{(3)}\) measurements indicate however, that the spin reorientation is spread over an interval of temperature. The purpose of the present study was to make use of the neutron diffraction technique to gain more insight into the nature of the spin reorientation taking place in rare-earth iron Laves compounds.

A powder specimen of composition \( Ho_{0.6}Ta_{0.4}Fe_2 \) was used for the neutron diffraction studies. The powder was mixed with a self-curing resin and the mixture allowed to harden in a 25 kOe magnetic field. Neutron diffraction was performed in the temperature range 4.2°-300°K and the following results obtained:

a) The sample is fully aligned in the [111] direction.
b) The [111] intensity-temperature curve obtained with no external magnetic field is smooth and similar to the curve observed for \( ErFe_2 \) \(^{(4)}\), which
does not exhibit spin reorientation. This is expected in multidomain cubic crystals where intensities are independent of the spin direction. c) In an internal 7 kOe field, however, the [111] intensity-temperature curve exhibits an anomaly in the 700-1400 K range. This anomaly is interpreted as a spin reorientation from the [111] to the [110] direction.

The present results were fitted to a continuous spin reorientation and the direction of the magnetization determined as a function of temperature during reorientation.

REFERENCES:

DETERMINATION OF GRAIN SIZE IN U-Cr ALLOYS BY ULTRASONIC ATTENUATION MEASUREMENTS
J. Roman *, M. Oron *, J. Pesach ** and M. Rosen

Ultrasonic attenuation was measured in cylindrical samples of uranium-chromium alloys. The grain structure of the samples was previously refined by heat treatment, and grain size in the range of 50 to 200 um was determined by conventional metallographic methods. The attenuation coefficient was correlated with the mean grain diameter for three ultrasonic frequencies, 4 MHz, 6 MHz and 12 MHz. The experimental results were compared with existing theories and good agreement was found with the curves based on Merkulov's analysis for cubic metals.

A practical result of this work was the development of a nondestructive testing procedure for grain size determination. The highest frequency (12 MHz) is normally used as it is more sensitive in the lower grain size range (50-100 μm) and only in borderline cases are the lower frequencies preferred, particularly for grain sizes 200 μm.

REFERENCE:

* Hebrew University, Jerusalem
** Morex 71, Ltd., Tel Aviv
TEMPERATURE DEPENDENCE OF THE ELASTIC MODULI OF POLYCRYSTALLINE ZrZn$_2$

G. Dublon, M. Rosen, M. Weger, and Z. Kalman

The longitudinal and transverse sound velocities in the weak itinerant ferromagnet ZrZn$_2$ were measured as a function of temperature between 10$^\circ$ and 300$^\circ$K. The temperature dependence of the Young and shear moduli, the Debye temperature, and the adiabatic compressibility were calculated. Two anomalies were observed: one at 220$^\circ$K, which may be accounted for by the anisotropic d-band structure of ZrZn$_2$; the second at 45$^\circ$K suggesting a first-order phase transition the nature of which is not yet understood. No significant change in the elastic moduli was observed at the Curie temperature.

REFERENCE:

SOUND VELOCITY AND ULTRASONIC ATTENUATION ANOMALIES IN LIQUID Bi-Ga ALLOYS WITH A MISCELLIBILITY GAP

Z. Salton, M. Rosen and B.Z. Weiss

The temperature dependence of the sound velocity and ultrasonic attenuation in several liquid bismuth-gallium alloys was determined by means of an ultrasonic pulse technique. A rapid gravitational phase separation was observed at 262$^\circ$C for the critical composition, Bi - 43.77 $\%$ Ga. Ultrasonic attenuation measurements permitted the accurate determination of the position of the interface (meniscus) between the separated liquid phases. The rate of motion of the meniscus as a function of temperature and composition was measured.

REFERENCE:

TRANSFORMATION TWINS AND THE ELASTIC PROPERTIES OF U$_3$Si AT LOW TEMPERATURES

M. Rosen, Y. Gefen, G. Kimmel and A. Halwany

The elastic properties, adiabatic compressibility and Debye temperature of twinned and non-twinned U$_3$Si were determined between liquid helium and ambient temperatures by means of an ultrasonic pulse technique. The twinned
and non-twinned face centered tetragonal \( U_3Si \) specimens were prepared employing appropriate heat treatment regimes. The presence of twins in the \( U_3Si \) lattice yields a modulus defect of about 18.5%, the Young's modulus of the twinned \( U_3Si \) having the lower absolute value. At about 85\( ^0\)K the twinned structure displays a prominent minimum in its elastic properties, suggesting a first order phase transformation. In contrast, the non-twinned \( U_3Si \) exhibits a maximum in this temperature range. The experimental results were analyzed in terms of the effect of twins on the lattice stability of the tetragonal structure of \( U_3Si \).

REFERENCE:

SINGLE CRYSTAL ELASTIC CONSTANTS AND MAGNETOElasticITY OF HOLMIUM FROM 1.2\( ^0\) O TO 300\( ^0\)K(1)

M. Rosen, D. Kalir and H. Klimker

The five independent elastic coefficients of holmium single crystals were determined by means of an ultrasonic pulse technique at a frequency of 10 MHz, between 4.2\( ^0\) and 300\( ^0\)K. From the elastic constants the temperature variation of the directional adiabatic compressibilities, the limiting Debye temperature and the elastic anisotropy ratio were calculated. The elastic coefficients exhibit anomalies at the magnetic ordering transitions known to occur in holmium. Anomalous behavior in the elastic constants was also observed at about 80\( ^0\)K. The limiting value of the Debye temperature was found to be 191.5\( ^0\)K. The present measurements of the elastic constants, and the reported magnetostriction and thermal expansion data permitted the calculation of the magnetoelastic contribution to the total hamiltonian of holmium in the magnetically ordered states. A very small discontinuity in the temperature dependence of the magnetoelastic energy was observed at the Curie point of holmium. Below the Neel temperature, the magnetoelastic energy varies smoothly with decreasing temperature, attaining a value of \(-2.13\) J cm\(^{-3}\) at liquid helium temperature. The temperature dependence of the magnetoelastic energy in the vicinity of the Curie point in holmium suggests that the magnetic transition from the antiferromagnetic arrangement into the ferromagnetic state is of second order.

REFERENCE:
CONTROL OF GRAIN SIZE IN URANIUM-CHROMIUM ALLOYS BY HEAT TREATMENT

J. Roman*, M. Oron* and M. Rosen

A parabolic relationship was found between the β → α transformation temperature and the grain size.

REFERENCE:

MECHANISMS AFFECTING MECHANICAL PROPERTIES OF URANIUM BASE ALLOYS

A. Arbel

Considerable efforts have been made to alloy uranium in order to improve its mechanical properties for structural and radiation shielding applications.

This study was undertaken in order to investigate the mechanisms affecting mechanical properties of polynary uranium alloys. Several successful castings were made of uranium containing Mo, Zr, Nb and Ti. Specimens were solution treated at 950°C in evacuated quartz tubes and water quenched, which resulted in a hardness of 200 DPH. Aging at 270°C-320°C resulted in a hardness of 550 DPH. The changes in the microstructure responsible for hardening will be studied with the aid of optical and electron microscopy.

REFERENCE:

BULK MAGNETIC ANISOTROPY CONSTANTS OF THE RARE-EARTH IRON LAVES COMPOUNDS

M. P. Dariel and U. Atzmony

The one-ion model satisfactorily accounts for the magnetic anisotropy properties of the rare-earth iron Laves compounds. The bulk anisotropy constants $K_1$ and $K_2$ in the temperature interval 4.2-300°K, were calculated for the $\text{RFe}_2$ compounds, R=Tb, Dy, Ho, Er and Tm.

REFERENCE:

* Hebrew University, Jerusalem
SPECIFIC HEAT ANOMALIES AT THE ORDERING TEMPERATURES OF RARE-EARTH IRON LAVES COMPOUNDS\(^{(1)}\)
M.P. Dariel, U. Atzmony and R. Guiser

The magnetic ordering temperatures of rare-earth and yttrium iron Laves compounds were determined by measuring the specific heat anomalies in a differential scanning colorimeter. The results are in general agreement with those deduced from magnetization measurements. The specific heat discontinuities at the magnetic ordering temperatures are not consistent with the theoretical expressions derived for ferrites.

REFERENCE:

ELASTIC AND MAGNETIELASTIC PROPERTIES OF RARE-EARTH IRON LAVES COMPOUNDS
H. Klimker, M. Rosen, M.P. Dariel and U. Atzmony

The temperature and magnetic field dependence of the elastic moduli and adiabatic compressibility of a series of rare-earth iron Laves compounds \(\text{RFe}_2\) (\(\text{R} = \text{Y, Ce, Gd, Tb, Dy, Ho, Er}\)) was determined. The importance of the magnetoelastic effects in the series was evaluated. Anomalies in the elastic moduli and the significant \(\Delta\varepsilon\) effects observed particularly in \(\text{TbFe}_2\) were correlated with the magnetic properties of the compounds.

REFERENCE:

ELECTROMIGRATION OF Ag AND Zn TRACERS IN PRASEODYMIUM\(^{(1)}\)
A. Tessler and M.P. Dariel

The steady state method was used to study the electromigration of silver and zinc tracers in praseodymium.

The silver tracers migrated towards the cathode with an effective charge \(Z^* = 1\), while \(Z^*\) of the zinc tracers was close to zero. These results suggest that the diffusion of these solutes does not take place by a purely interstitial mechanism.

REFERENCE:
The magnetic properties of the weak itinerant ferromagnets (Zr$_{1-x}$Hf$_x$)$_2$Zn$_2$ and (Zr$_{1-y}$Ti$_y$)$_2$Zn$_2$ have been extensively studied. It was suggested that the large variations of the Curie temperature $T_C$ and the magnetization $M$ with either the Hf or Ti content are due to changes in the exchange interaction parameter $J$. Another quantity which dominates the magnetic properties of itinerant ferromagnets is the density of states function $n(E)$, which in ZrZn$_2$ consists of a sharp and narrow d-band peak at the Fermi level.

We made magnetic susceptibility measurements of (Zr$_{1-x}$Hf$_x$)$_2$Zn$_2$ compounds ($x,y = .05 - .20$) as a function of temperature (4.2-300°K) and magnetic field (7-16 kOe).

Simple theory assumes that both Hf and Ti affect the average properties which dominate the tendency to itinerant ferromagnetism. As such, Hf and Ti will contribute additively to $T_C$ and $M$. It was found, however, that Hf mainly affects $M$ and its field dependence, whereas Ti determines $T_C$.

Since, for a simple model based on the RPA, $T_C$ depends mainly on $n(E_F)J$ and $M$ depends mainly on $n(E_F)\delta E$, $\delta E$ being the width of the peak in the density of states function, it is conceivable that Ti mainly affects $J$ and Hf mainly affects $\delta E$.

REFERENCES:

A MICROSECTIONING TECHNIQUE FOR VANADIUM

J. Pelleg

Thin sections can be removed from vanadium metal by a combined anodizing and stripping technique. A uniform, thin oxide film was grown on vanadium metal in an acetone - benzoic acid - sodium tetraborate solution during anodization, which was then removed in aqueous NH$_4$OH (10%). The thickness $x$ of the metal removed in angstrom units is given by $x = 103.2+12.5 \, V$, where $V$ is the applied voltage. The application of such a sectioning technique

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MAGNETOELASTICITY IN SmFe₂
M. Rosen, H. Klimker, U. Atzmony and M.P. Dariel

The temperature and magnetic field dependence of the elastic moduli of SmFe₂ Laves phase compound was investigated by means of an ultrasonic pulse technique at a frequency of 10 MHz. The spin reorientation from the high temperature easy direction of magnetization [111] to the low temperature easy axis directed along [110] was observed to occur at Tₑₘₐғ = 195ºK. The behavior of the elastic moduli near Tₑₘₐғ suggests a first-order phase change. Applied magnetic fields strongly affect the temperature dependence and the absolute values of the elastic moduli of SmFe₂. The elastic moduli increase significantly with increased magnetic fields, yielding a low temperature-independent adiabatic compressibility. A remarkably high (42%) ΔE effect was observed in SmFe₂ at room temperature, 10 MHz ultrasonic frequency, and an applied magnetic field of 25 kOe. The magnetostriction of SmFe₂ is high and negative. For a field of 25 kOe at room temperature and 77ºK, values are -2,100 and -3,400 x 10⁻⁶, respectively. The limiting values of the Debye temperatures were found to be 200º and 212ºK, for unmagnetized samples and those in a 25 kOe field, respectively.

REFERENCE:

MAGNETIZATION OF ORDERED SmFe₂
G. Dublon, U. Atzmony and M.P. Dariel

The magnetic properties of Sm³⁺-bearing materials are noted for their complexity as compared with other tripositive rare-earth (RE) compounds:

a. The 4f-induced Knight shift of ⁷¹Al in paramagnetic SmAl₂ does not exhibit a sign reversal as predicted by Van Vleck (1).

b. The magnetic moment of Sm³⁺ in some intermetallics is found to be substantially lower than the free-ion moment (2).

c. Among the cubic Laves RE iron compounds, SmFe₂ is the only purely binary material to possess a temperature dependent easy direction of magnetization (3,4).
Much of this complexity is attributed to the fact that the energy separation between the ground ($J = 5/2$) and first excited ($J = 7/2$) multiplets of Sm$^{+3}$ is small enough (14000 K), so that crystal and exchange fields may mix the excited into the ground state\(^{(1-3)}\). Thus, it is suggested\(^{(1)}\) that Sm$^{+3}$ might show L+S instead of the usual L-S behavior of all other light RE ions. In suggesting such a change of sign of $<S_z>$ in SmFe$_2$ while accounting for the observed spin reorientation in this material, fourth and sixth-order crystal fields are taken to be of the same order of magnitude\(^{(3)}\). This contradicts the appreciably lower $A_6/A_4$ ratio found in all the other cubic Laves RE iron compounds\(^{(4)}\).

In the present work, magnetization measurements of powdered SmFe$_2$ ($T_c = 700^\circ$K) were made as a function of temperature (4.2$^\circ$-300$^\circ$K) and magnetic field (1-15 kOe) using a null coil pendulum magnetometer. The main features of the results obtained are:

a. As the temperature is increased an appreciable increase in the magnetization ($M$) is observed around 80$^\circ$K in all applied magnetic fields. At higher temperatures $M$ decreases smoothly.

b. The moment observed at 80$^\circ$K (15 kOe) is 2.2$\mu_B$ per unit formula, whereas at 4.2$^\circ$K (15 kOe) it is about 1$\mu_B$ lower.

This may be indicative of a ferrimagnetic ordering in SmFe$_2$ in which the moment of Sm$^{+3}$ differs from its free-ion value. It is believed that the observed anomalies may be accounted for by crystal field effects. The appropriate theoretical calculations are in progress.

REFERENCES:

PHASE TRANSFORMATION IN SOME RARE-EARTH HYDROGEN SYSTEMS\(^{(1)}\)
M.H. Mintz, Z. Hadari and M. Bixon

The range of stability of Pr, Nd and Sm hydrides was investigated using simultaneous TG-DTA techniques. Measurements were made over a temperature range 25$^\circ$-700$^\circ$C, at 700 Torr hydrogen pressure. A new low temperature
hexagonal phase was detected in the NdH₂ - NdH₃ system. Its structure is similar to the hexagonal, heavier lanthanide hydride phases. However, unlike these structures the NdH₂₋ₓ hexagonal phase transforms irreversibly on heating to the fcc structure which remains metastable at room temperature. The enthalpy changes associated with the hexagonal to fcc transitions in the NdH₂ - NdH₃ and SmH₂ - SmH₃ systems were estimated to be 1.6 ± 0.3 kcal/mole and 4 ± 0.4 kcal/mole, respectively. No phase transition was detected in the PrH₂ - PrH₃ system.

REFERENCE:

HYDROGEN BLISTERING OF TECHNICAL ALUMINUM
M. Zafrir, D. Kedem and A. Aladjem

The formation of hydrogen blisters on technical aluminum and aluminum alloys as a result of improper heat treatment, the presence of impurities in the atmosphere, etc., is a well-known phenomenon that occasionally causes great damage to heat-treated aluminum components.

A series of closely controlled experiments was carried out to establish the relative contribution of different factors to the formation of blisters on technical aluminum during a heat treatment process.

The specified heat treatment was 5 hours at 530°C in air. Specimens were taken for treatment: (a) after machining and degreasing, (b) after machining, degreasing and etching in a hot alkaline solution and (c) after machining, degreasing and chemical oxidation of the surface.

The following factors were tested:
(1) temperature deviations during heat treatment in the range 480°C - 570°C
(2) increased treatment time to up to 16 h
(3) variations in the cooling rate after the heat treatment, from very rapid quenching to cooling
(4) variations in the time between the machining or etching and the heat treatment, from a few minutes to one month
(5) variations in the alkaline etch solution (NaOH, Na₃PO₄)
(6) introduction of water vapor, trichloroethylene vapor or ammonia into the furnace atmosphere during the heat treatment.
None of the above factors, except (1), caused the appearance of blisters on the surface of the heat treated samples. The influence of temperature was pronounced; on samples of types (a) and (b), blisters appeared in all cases in which the temperature exceeded 560°C, while on samples of type (c) the blisters were formed upon heat treatment above 570°C. In all cases the blisters appeared mainly on surfaces exposed to the air, while surfaces in contact with the refractory were fairly free of blisters.

The results indicate that the appearance of blisters requires a combination of at least two factors—temperatures above specified values, and surface contact with air. It is, however, conceivable that certain impurities in the atmosphere (e.g., reagents that promote the diffusion of protonated hydrogen into the metal rather than the evolution of molecular hydrogen) could cause hydrogen blistering even at the specified temperature.

CORROSION OF COPPER, NICKEL AND IRON IN ALPHA-RADIATION FIELDS
G. Gafny and A. Aladjem

The adequate selection of structural metals for service in the presence of alpha radiation requires a knowledge of the corrosion resistance of the proposed metals, both in the case of direct impingement of the energetic alpha particles on the metal surface (i.e., direct effect) and in the case of exposure of the metals to alpha-radiolysis products in the environment (i.e., indirect effect). Such radiolysis products are often strongly oxidizing or reducing species and although short-lived their diffusion in gases is very rapid and their effect could be observed at distances much beyond the alpha-particle range in the gas.

In a series of tests we examined the direct and indirect effects of 5.4 MeV alpha radiation from 40mCi $^{241}$Am sources on the corrosion of technical-grade copper, nickel and iron strips in air saturated with H$_2$O and trichloroethylene vapors, at room temperature. Trichloroethylene was introduced to enhance the indirect effect, since it is well known that in the absence of radiolysis its vapors do not accelerate corrosion of Cu, Ni and Fe.

The irradiation was carried out over 80 days, with periodic checks of surface condition and weight. At the end of that period, the nickel surface remained unchanged and there were negligible changes in weight. The copper surface lost its lustre and there were many dark-brown spots, while the entire iron surface was rusted. The surfaces of all unirradiated samples remained unchanged.
Quantitatively, the effect of radiation is expressed in terms of the radiation corrosion (rc) enhancement factor $K_{rc}$

$$K_{rc} = \left(\frac{\Delta g_i}{a_i}\right) / \left(\frac{\Delta g_s}{a_s}\right)$$

where $\Delta g_i$ and $\Delta g_s$ are the changes in weight of the irradiated and non-irradiated (standard) samples respectively, and $a_i$ and $a_s$ are the respective surface areas. The values of $K_{rc}$ are given in Table 1.

**TABLE 1**

<table>
<thead>
<tr>
<th>Test time</th>
<th>Copper</th>
<th>Iron</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>direct effect</td>
<td>indirect effect</td>
</tr>
<tr>
<td>20 days</td>
<td>5</td>
<td>3</td>
</tr>
<tr>
<td>80 days</td>
<td>11</td>
<td>3</td>
</tr>
</tbody>
</table>

The results indicate that: (a) the resistance of nickel was not affected by the radiation; (b) copper and iron were altered in the presence of radiation, and there were substantial direct and indirect effects; (c) the direct effect on iron decreased sharply with time, assumably because of the radiation shielding effect of the oxide film.

DEVELOPMENT OF CRITERIA FOR EVALUATING THE SUSCEPTIBILITY OF ALLOYS TO STRESS CORROSION CRACKING

A. Aladjem

Two criteria for evaluating the susceptibility of structural alloys (e.g. high-strength Ti alloys for aircraft use, corrosion-resistant zirconium alloys for use in nuclear technology, etc.) to stress corrosion cracking (SCC) were established on the basis of theoretical considerations and experimental work.

A simplified model of the SCC process was used as a basis for the criteria. It was assumed that the process involves two stages, i.e., (1) an incubation step of penetration of the passivating oxide layer on the surface and development of a "critical" crack, and (2) a crack propagation stage. The two stages are distinct and separate, and a different susceptibility criterion was established for each of them.
In experimental work on the SCC of metals, the long times associated with the first, incubation step, are usually eliminated by fatigue pre-cracking of the specimen; thus most experimental data refer to the second step alone.

For the first stage, it was assumed that the ease of penetration of the passivating oxide film was inversely proportional to its apparent polarization stability. The stability was measured by applying a very high electric field, of the order of $10^6$-$10^7$ volts/cm, across the film. The specimen was anodically polarized and under these conditions a current of a few $\mu$A/cm$^2$ or less passed from the specimen to the electrolyte, provided that a non-corrosive electrolyte was used. Any change in conditions caused a measurable change in the current, i.e., the addition of a corrosive agent, or improper heat treatment of the alloy, or external stress increased the current, while addition of corrosion inhibitors, stress relief, etc., reduced the current. An arbitrarily quantitative, dimensionless criterion for the susceptibility to SCC under changing conditions was thus established: $S_{\text{scsi}} = I_e/I_p$ where $S_{\text{scsi}}$ is the susceptibility criterion for the incubation step, $I_e$ is the current under the changed conditions and $I_p$ is the current under the "passivated" condition. Earlier work on a Ti-Sn-Al alloy supports the adequacy of the above criterion.

For the second stage, it was assumed that crack propagation is unequivocally associated with hydrogen accumulation in the sample. This is again a simplification, but it is a well established fact that hydrogen accumulating at the crack tip is a major factor promoting the crack propagation (for instance, failure of Zircaloy claddings of nuclear fuel is usually attributed to hydriding of the Zircaloy). The relative tendency to absorb corrosion-generated hydrogen was measured by cathodically polarizing the specimen in an electrolyte, preferably similar to the one used as the actual service medium. The amount of hydrogen absorbed by the sample $Q_{\text{Ha}}$ was then related to the amount theoretically evolved on the specimen ($Q_{\text{Ht}}$), as calculated from Faraday's law on the basis of a measurement of the integrated current. The crack-propagation susceptibility criterion was then formulated: $S_{\text{scp}} = Q_{\text{Ha}}/Q_{\text{Ht}}$.

For both stages of the process, an increase in the absolute value of the criteria indicated an increase in susceptibility to SCC. The overall criterion for the influence of a change in conditions on the SCC of an alloy would be $S_{\text{sc}} = K S_{\text{scsi}} S_{\text{scp}}$, where $K$ is a constant whose value depends on the material used.

REFERENCES:
2. Scott, R., Nucl. Safety 14, 507 (1973)
ELECTRON MICROSCOPY OF U₃Si
G. Kimmel, U. Admon, E. Nehama and B. Yusuf

Thin foils of martensitic U₃Si were examined under the electron microscope before and after rolling. Double stage replicas were used to observe surfaces after fracture.

U₃Si, which had been cooled from 850°C to room temperature, revealed a twinned structure as a result of the martensitic transformation $\delta' \rightarrow \delta$. After rolling, the microtwins could not be observed under T.E.M. This conforms with previous results found by X-ray diffraction and by optical metallography.

A comparison between martensitic and non-martensitic specimens after fracture shows that the microtwins do not play any role in the fracture mechanism of U₃Si. The fracture found was always intercrystalline. Since the traces of the cleavage planes form a pattern of squares, it is supposed that the cleavage planes are {100} and {110} in bct and {001} and {100} in fct U₃Si.

POSITRON ANNIHILATION IN A SINGLE TiO₂ CRYSTAL
D. Tsur, M. Blau and M. Weger

Positron annihilation in a single crystal of rutile (TiO₂) was investigated by analyzing the energies of the emitted $\gamma$-rays. The anisotropy in the energy distribution for emission parallel and perpendicular to the crystal c-axis was measured and found to be $2.3 \pm 0.3\%$ for $k=0$, and to vanish at $k=3.7 \pm 0.3$ mrad, where $k$ is the resultant positron-electron momentum. The anisotropy is attributed to covalency of the oxygen 2p shell. Thus, this method provides a novel way to estimate and compare the covalency of partly ionic crystals.

REFERENCE:

PREPARATION AND PROPERTIES OF SINGLE CRYSTALS AND THIN FILMS OF SbSI
M. Barkai, P. Buchman and S. Szapiro

SbSI needle crystals, 4 cm long and 2 mm$^2$ cross section, were grown in an evacuated pyrex ampoule in a two-zone furnace at temperatures of 410°C and 360°C. These crystals exhibit ferroelectric properties with a Curie temperature of 20°C, a spontaneous polarization $P_s$ of 20 $\mu$C/cm$^2$ and a peak dielectric constant of 16,000.
Attempts were made to obtain a thin film of SbSI by the standard technique of evaporation and sputtering. The instability of the material, however, resulted in the deposition of decomposed layers. Encouraging results were obtained by melting SbSI crystals between two pressed glass substrates in an argon and SbI$_3$ atmosphere, and then quenching. The resulting film shows X-ray lines characteristic of SbSI with an optical absorption edge of 1.9 eV. Although the material does not exhibit ferroelectric properties, the dielectric constant is \( \sim 1000 \) with a resistivity of \( 10^8 \) ohm-cm. The film is photoconductive, independent of temperature.

REFERENCE:
Laser induced thermonuclear fusion is one of several research areas which have led to an interest in developing high energy, short pulse lasers. Various theoretical calculations predict that the thermonuclear energy release exceeds the input laser energy when irradiating submillimeter diameter spheres of deuterium-tritium mixtures by a properly tailored laser pulse having an energy of about $10^4$ joules (1-4).

A high power Nd:glass laser facility has been constructed and is now in operation. The facility consists of a passively mode-locked Nd:glass oscillator generating pulses of $10^{-10}$ sec (Fig. 1) followed by a selection stage, where a set of 2 Pockels' cells, placed alternately between 3 polarizers, are activated by a laser triggered spark gap, admitting a single pulse into the amplifier cascade (Fig. 2). The single short pulse is amplified by 6 amplifiers in series. A schematic diagram of the system is shown in Fig. 3 and a photograph of the oscillator and first amplifier stage is shown in Fig. 4. A total energy of a few tens of joules is obtained at the output of

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**Fig. 1**
A mode-locked train of the Nd:glass oscillator as monitored by an HP 4220 photo-diode and Tektronix 485 oscilloscope. A 12 ns time delay between subsequent pulses is determined by oscillator cavity length.

**Fig. 2**
A typical single pulse selected from the mode-locked train. This pulse is admitted to the amplifier cascade of the system. The oscilloscope time base is the same as presented in Fig. 1.
Fig. 3
Schematic diagram of the laser system

Fig. 4
Photograph of the oscillator, switching stage and first amplifier of the system
the last amplifier. The characteristics of the amplifier system are given in Table 1.

**TABLE 1**
Amplifier system characteristics

<table>
<thead>
<tr>
<th>Head</th>
<th>Diameter (inch)</th>
<th>Length (inch)</th>
<th>Rated pump energy, kJ</th>
<th>Input energy</th>
<th>Output energy</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amp I</td>
<td>0.75</td>
<td>16</td>
<td>3.5</td>
<td>0.5-1.0 mJ</td>
<td>20-40 mJ</td>
<td>Divergence limiting aperture</td>
</tr>
<tr>
<td>Amp II</td>
<td>0.75</td>
<td>16</td>
<td>3.5</td>
<td>1.0-2.0 mJ</td>
<td>40-80 mJ</td>
<td></td>
</tr>
<tr>
<td>Amp III</td>
<td>1.0</td>
<td>16</td>
<td>4</td>
<td>40-80 mJ</td>
<td>0.4-0.8 J</td>
<td>Pulse stretching system</td>
</tr>
<tr>
<td>Amp IV</td>
<td>1.0</td>
<td>16</td>
<td>4</td>
<td>0.2-0.4 J</td>
<td>2-4 J</td>
<td></td>
</tr>
<tr>
<td>Amp V</td>
<td>1.5</td>
<td>20</td>
<td>15</td>
<td>2-4 J</td>
<td>10-20 J</td>
<td></td>
</tr>
<tr>
<td>Amp VI</td>
<td>2.0</td>
<td>20</td>
<td>20</td>
<td>10-20 J</td>
<td>50-100 J</td>
<td></td>
</tr>
</tbody>
</table>

The values of input and output energies for each amplifier are based on small signal gain measurements performed on each amplifier module. Total output power of the system is limited at this stage by the self-focusing damage threshold which is considered to be as low as 5x10^9 watts/cm^2 of average energy density. This last number depends essentially on the beam quality of the system. Therefore, much effort is directed at improvement of the beam quality of the system. Temporal pulse length of the oscillator can be varied with the aid of an intracavity etalon.

After passing the amplifiers the light pulse is directed into the reaction chamber where it is focused onto a 30 μm diameter spot by an aspheric lens. The target chamber is equipped with target insertion and positioning equipment as well as 16 diagnostic ports.

The system is operated from a central control room and is able to produce a pulse every 5 minutes.

**REFERENCES:**
PREPARATION OF TARGETS FOR LASER-INDUCED PLASMA EXPERIMENTS
I. Lewkowicz, Y. Haruvi and S. Shamash

Research on hydrogen plasmas for nuclear fusion reactions requires that a spherical deuterium target be placed at the focus of the laser beam. Because of technological difficulties in producing small solid deuterium spheres, such targets have not been used, and instead deuterium ice cylinders or spherically shaped deuterium compounds (1) were used. Although the latter are not optimal for fusion experiments because of the presence of nonfusile atoms in the sphere, much data has been reported using these targets. Using newly developed techniques, we have also produced small solid spheres from lithium deuteride and deuterated polyethylene. Electron photomicrographs of targets obtained are shown in Figs. 5 and 6.

In an attempt to obtain a more ideal target we have evaluated the possibility of using commercially available borosilicate glass microballoons as containers for hydrogen isotopes (Fig. 7). The permeability of hydrogen into such balloons and their mechanical strength were calculated. The fraction of external pressure that accumulates in the microballoon at various temperatures as a function of time is shown in Fig. 8. The maximum difference between the external and internal pressure that a microballoon can suffer without crushing is given in Fig. 9 as a function of the radius of a microballoon.

The experiments were carried out using the apparatus shown in Fig. 10. Microballoons, graded according to size, were placed in an autoclave (A). The autoclave was evacuated and a hydrogen pressure of 50 atm applied. The pressure was raised stepwise in order to maintain the maximum pressure gradient without breaking the balloons. After equilibration (see Fig. 8), the autoclave was cooled to liquid nitrogen temperature and connected to a vacuum system, evacuated when cold and then warmed up to 400°C to release accumulated hydrogen in the microballoons. The maximum pressure inside the microballoons was calculated to be 250 atm.

Thus we devised a new, relatively simple and reliable technique for the preparation of high pressure hydrogen targets. In principle it should be possible to improve the targets by liquefying the hydrogen inside the microballoons, thereby obtaining higher densities at lower pressure. The advantage of these targets lies in the fact that they have a well-defined spherical shape and may be filled with fusile material.
Fig. 5
Lithium deuteride sphere, 100 μm diam

Fig. 6
Deuterated polyethylene sphere, ×3000X

Fig. 7
Glass microballoons, 100 μm diam
Fig. 8
Growth of the pressure inside the microballoons (expressed as the ratio of internal to external pressures) as a function of time for various temperatures.

Fig. 9
Maximum allowable pressure inside the microballoon as a function of its radius for three different rupture strengths $S$.

Fig. 10
Apparatus for high pressure experiment.

REFERENCE:
1. Friedman, W.D., Halpern, G.M. and Brinker, B.A., Target fabrication and positioning techniques for laser fusion experiments, University of Rochester, Report No.22.
Vacuum Photodiode Holder for Laser Plasma Diagnostics
S. Eckhouse, B. Divon and Moshe Oron

High speed vacuum photodiodes were tested for future use as monitors in the laser plasma diagnostic setup. Optimum time response is expected only if suitable photodiode holders are used.

Figure 11 is a cross section of the photodiode mount designed for accommodating I.T.T. type F4000 (or FW114A) photodiodes. Positive high voltage is applied to the anode, thus buffering the recording setup from the high voltage circuitry. Time domain reflectometry measurements, using the Hewlett-Packard model 1415A system, demonstrated reflection coefficients of less than 10%, if the holder was terminated by a mesh of ten 500Ω parallel resistors, in place of the photodiode. For this accuracy, the holder is assumed to exhibit a 50Ω line between the photodiode and the transmission line. Thus, the rise-

Fig. 11
2" Photodiode holder

1. Charging capacitor 6. Outer conductor
2. HV connector 7. Inner conductor
3. RTV potting 8. Photocathode
4. 10 MΩ HV resistor 9. ITT photodiode
5. 50Ω output connector
time of the photodiode and the transmission line is expected to be of the order of 350 psec\(^{(1,2)}\). The photodiode time response was also tested as a function of the bias voltage, up to 6 kV, with negligible noticeable effect. Saturation current densities of the order of \(2 \times 10^2\) were measured at 6 kV bias voltage. The deviation of the dependence of saturation densities on voltage from the \(v^{3/2}\) law was less than 20%.

REFERENCES:

LINEAR OUTPUT CURRENTS OF SOME PHOTOMULTIPLIER TUBES
B. Divon, S. Eckhouse and Y. Komet

Light measurement for plasma diagnostics is characterized by a high dynamic range of light fluxes. Increasing the dynamic range of photodetectors for such purposes may, therefore, be important.

An experimental setup for measuring the linear currents of PM tubes is given in Fig. 12. The pulsed light source is an EGGFx33C2 flashlamp having a pulse width of \(\sim 10\)\(\mu\)sec. The pulse shape is measured by a PM monitor, which is linear over the full pulse width. The output of this monitor is fed into

![Fig. 12](image)

Setup for photomultiplier linearity measurement
the x-input of an x-y oscilloscope. The output of the tested PM is fed into the y-input, and the anode linear current range is deduced from the photograph of the CKT trace. The trace is z-modulated by the pulse of the flashlamp in order to reduce the light background. Suitable changes in the voltage dividers of Philips type 56AVP and XP2020 photomultipliers and the EMI 9597QB PM resulted in a three-fold improvement in the linear currents, as compared with the currents quoted in the data sheets. Figure 13 is an example of a voltage divider for a 56AVP photomultiplier, from which linear currents of the order of 0.9A, with a 5% deviation from linearity, were obtained at -2500V working voltage.

Fig. 13
Voltage divider for a high linear current from a 56 AVP photomultiplier

CURRENT PROBES AS A DIAGNOSTIC METHOD FOR STUDYING PLASMA
M. Loebenstein

One of the simplest diagnostic methods is to measure the current pulse of expanding plasma particles by means of current probes. For pure hydrogen targets the current pulse gives the energy and the number of the charged particles by means of the time-of-flight method. For heavier or composite targets, where different ions of various ionization states emerge, additional information has to be obtained from the e/m spectrometer in order to analyze the current pulse. Also by placing current probes around the target, information is obtained about the angular distribution of the expanding plasma and whether the laser hit the target at the center. The latter is one of the crucial criteria in deciding whether the shot was a "good" one.
MEASUREMENTS OF MOMENTUM OF PARTICLES EMITTED FROM LASER-PRODUCED PLASMA

M. Kuznietz

Microphones (starting with a foil-electret microphone in its electrostatic mode) are being used to measure the time integrated momentum flux of particles, charged as well as neutral, emitted from plasmas produced in various targets by our short-pulse high-power Nd:glass laser. The ac pulse obtained depends on the characteristic restoring time of the microphone, in the case where the particle arrival times are much shorter than this restoring time. The pulse height is proportional to the momentum delivered by the particles. Special attention is given to the response of the microphone to X-ray and scattered laser light.

X-RAY DIAGNOSTIC MEASUREMENTS OF LASER-PRODUCED PLASMA

D. Saltzman, H. Zmora and G. Ben David

X-ray diagnostic measurements are being carried out in four main areas:

1. An assembly of four silicon solid state detectors for measurement of plasma temperature by the absorption technique has been constructed and placed in the target chamber. The output pulses of the detectors are amplified, integrated, digitized and fed directly into the computer for on-line analysis.

2. An X-ray photographic plate holder is under construction. It will be used in integral measurements of X-rays and for pin-hole X-ray photography. The pin-hole camera itself is also under construction.

3. A high resolution grazing incidence grating spectrograph is being developed by the Hebrew University. It will permit spectroscopic measurements of soft X-rays in the range 5Å - 100Å, with an accuracy of one part in 2000. This spectrograph will be used for measuring spectral line intensities and line widths from the plasma.

4. TL detectors are being used for measurement of plasma temperature. Angular distribution measurements of the emitted X-rays will be attempted as well.

MEASUREMENTS OF NEUTRONS FROM LASER PRODUCED PLASMA

Y. Gazit

The thermonuclear reactions occurring in D-D or D-T plasmas involve emission of 2.5 and 14 MeV neutrons, respectively. Measurements of their number and energy spectrum can yield valuable information on the plasma under investigation.
The neutron detector consists of a 5"x5" NE102 plastic scintillator, coupled to a 58AVP photomultiplier. It is placed about 20 cm from the plasma. The detector is now being calibrated with a (D,D) neutron generator utilizing the method developed by Loebenstein and Gazit. It is expected that a yield of $5 \times 10^3$ neutrons/pulse will enable us to determine the number of neutrons with an accuracy of better than 50%.

REFERENCE:

ON-LINE DATA ACQUISITION SYSTEM FOR THE LASER-PLASMA DIAGNOSTICS
H. Szichman

An on-line data acquisition system has been developed, consisting of a 2100 HP on-line computer with an 8K memory and peripheral equipment to various laser diagnostic experiments. Software has been written to perform data collection and data processing for the following equipment:

a) 2 transient recorders connected to charged particle detectors.
   b) an 8-fold ADC for integral measurements with charged particle detectors.
   c) a 4-fold ADC for integral measurements with solid state X-ray detectors.
   d) laser monitoring instruments.

Preliminary data analysis, and important parameters are printed out by the computer teletype, while the complete raw data are outputed on a fast paper tape to permit further analysis on the 370/165 IBM computer.

LASER HEATING OF A PLASMA BY INVERSE BREMSSTRAHLUNG
H. Yatom and Y. Shima

The non-quantum mechanical theory of Dawson and Oberman for inverse bremsstrahlung absorption coefficients, valid for low radiation intensities, was extended to include the case of high radiation intensities. When the more recent quantum mechanical approach of Seely and Harris was reformulated so as to afford comparison with our extension of the Dawson and Oberman theory, we found that the expressions for the rate of energy absorption become identical in the limit where the photon energy is small compared with the electron thermal energy. This limit encompasses the usual case when the photon wave-
length is of the order of a micron (glass laser) and the electron temperature is \(10^5\) K or higher (interesting plasma energies).

REFERENCES:

BEHAVIOR OF HIGHLY COMPRESSED FISSILE SPHERES
A.D. Krumbein

It has been suggested\(^{(2,3)}\) that the critical mass of a fissionable assembly can be reduced to such a degree by laser implosion techniques that a fission microexplosion becomes possible\(^{(4)}\). The analysis given by Winterberg\(^{(4)}\) was tested numerically and extended to include the three main fissionable isotopes, as well as a fissionable core surrounded by a deuterium blanket. The neutron yield as a function of time was also obtained for a number of cases.

The IBM-370 versions of the SNG\(^{(5)}\) and SNT\(^{(6)}\) neutron transport codes were used in the calculations. The 16 group Hansen-Roach neutron cross sections\(^{(7)}\) were employed throughout. Use of the 26-group Bonderenko set and the inclusion of anisotropic scattering for deuterium were found not to have an appreciable effect on the results. In the calculations, the maximum compressions computed for both uranium and deuterium by the Thomas-Fermi equation\(^{(8)}\) were used at first. Since such high compressions are not realistic and would occur at best only close to the center of the sphere, three regions of varying density, deduced from the calculations of Brueckner\(^{(3)}\) and Nuckolls\(^{(9)}\), were used in later computations.

For a sphere of pure fissionable material at 240 times normal density, theoretically the maximum density attainable\(^{(8)}\), the results showed as expected that the critical radius scaled approximately as the inverse of the density. The smallest critical radius (.02 cm) was obtained for \(^{239}\)Pu and the largest (.033 cm) for \(^{235}\)U, with \(^{233}\)U giving a value close to that of \(^{239}\)Pu. The critical masses range from about 0.7 g for \(^{235}\)U to about 0.15 g for \(^{239}\)Pu. The results for a sphere of \(^{239}\)Pu surrounded by a shell of deuterium give a critical radius of 0.002 cm for a shell thickness of 0.005 cm with commensurate values for a \(^{235}\)U core. These results no longer agree with Winterberg's simple analysis\(^{(4)}\), but give considerably smaller critical radii.
Time dependent calculations, performed with the SNT\(^6\) code, show that in order to achieve neutron multiplications of the order of \(10^{20}\), (necessary if such spheres are to serve as power sources), in the time it takes a \(^{239}\)Pu microsphere to come apart, (approximately \(10^{-9}\) sec), the critical radius must be multiplied by at least a factor of three. The moderated microsphere never attains high neutron multiplication rates due to the long transit times, (as compared with \(10^{-9}\) sec), of the moderated neutrons.

Spheres of \(^{239}\)Pu, for which the most optimistic compressions calculated in Refs. 3 and 9 were used, gave a critical radius more than 10 times as large as that for the maximum theoretical density, i.e.\(0.25\) cm for \(^{239}\)Pu. Replacing the outermost, or least compressed, layer of \(^{239}\)Pu by deuterium reduces this large value by a factor of about 3.

The foregoing results appear to indicate that only some sort of mechanism \(^{10}\) whereby fusion reactions, initiated in a D-T blanket by a microfissioning core, feed back neutrons to the fission process can make the use of fissionable microspheres at all feasible as a power source. Calculations are now underway in which this possibility is being investigated.

REFERENCES:
NUCLEAR PHYSICS AND CHEMISTRY
THE ROLE OF DISCRETE RESIDUAL LEVELS IN EVAPORATIVE DE-EXCITATION OF COMPOUND NUCLEI*
L. Segal and J. Gilat

In statistical model calculations particle evaporation from excited nuclei is usually represented by:

\[ R_{\mu}(E_c, J; E_f, j, s) = \frac{1}{\hbar} \frac{\rho(E_f, j)}{\rho(E_c, J)} \sum_{S = |j - s|}^{j + s} \sum_{E = |J - S|}^{J + s} T_{\mu E}(\epsilon) \]

where \( R_{\mu}(E_c, J; E_f, j, s) \) is the rate of emission of particle \( \mu \) (of spin \( s \)) from a nucleus with an excitation energy \( E_c \) and angular momentum \( J \) to form a residual nucleus with an excitation energy \( E_f \) and angular momentum \( j \); \( \rho(E_c, J) \) and \( \rho(E_f, j) \) are respectively the level densities of the initial and residual nuclei; \( \hbar \) is Planck's constant and \( T_{\mu E}(\epsilon) \) is the transmission coefficient for the inverse process, i.e. the reaction of particle \( \mu \) with an orbital angular momentum \( L \) and energy \( \epsilon(\epsilon = E_c - E_f - B; \ B \) is the binding energy of particle \( \mu \) in the initial nucleus) on the residual nucleus.

In most calculations this form is assumed to be valid even at low excitation energies (or near yrast), where the levels of the residual nucleus can no longer be described by a smooth level density function \( \rho(E_f, j) \). For a more realistic description of the excited nucleus one should use individual discrete levels, the spacing of which decreases with increasing excitation energy until they merge smoothly into a continuous level density function.

Such a model was incorporated into the spin dependent evaporation code GROGI 2 (1). The resulting new code (named GGL) was then applied to the calculation of cross sections and particle spectra for the reactions \( ^{62}\text{Ni}(p, p')^{62}\text{Ni}, \; ^{62}\text{Ni}(p, \alpha)^{59}\text{Co}, \; ^{59}\text{Co}(\alpha, \alpha')^{59}\text{Co} \) and \( ^{59}\text{Co}(\alpha, p)^{62}\text{Ni} \), at 18.06 MeV excitation energy of the \( ^{63}\text{Cu} \) compound nucleus. Results of the calculations were compared with experimental data, recently obtained by Miller and Jaffe. Good agreement between theory and experiment was achieved for very reasonable choices of input parameters. Miller and Jaffe (2) proposed (partial)

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*Based on the thesis submitted by L. Segal to Bar Ilan University in partial fulfillment of the requirements for an M.Sc. degree in chemistry.
conservation of isospin in these reactions, to explain some discrepancies between their measurements and conventional spin dependent statistical calculations. When we analyze the data with our improved and more realistic model, we find no evidence for such isospin conservation.

REFERENCES:

HIGH PRECISION STUDIES ON THE LEVEL SCHEME OF $^{80}$Se BY THE RESONANT-SCATTERING METHOD(1)
H. Szichman

The energies and reduced strengths of the $\gamma$-rays following deexcitation of the 7818.9 keV highly excited level in $^{80}$Se reached by the $(\gamma,\gamma')$ reaction were measured using a nickel capture $\gamma$ source. The level scheme deduced for this nucleus was given. Measurements of the angular distributions of the scattered radiation permitted the assignment of spin values for most of the low-lying levels in this nucleus. Parity determinations were made comparing the reduced strengths with the statistics of known $E1$ and $M1$ transitions.

REFERENCE:

$E1$, $M1$, $E2$ AND $M2$ WIDTHS OF TRANSITIONS FROM BOUND LEVELS EXCITED BY THE $(\gamma,\gamma')$ REACTIONS(1)
R. Moreh, A. Wolf, O. Shahal, and J. Tenenbaum

A comparison was made between the $E1$ and $M1$ transition strengths from bound levels populated by the $(\gamma,\gamma')$ reaction with the same data from unbound levels obtained via the $(n,\gamma)$ reaction. It was shown that there is a clear increase in the $M1$ strength nuclei near closed shells. The $E2/M1$ ratios were found to be of about the same magnitude as the Weisskopf estimate, while the $M2/E1$ ratios were enhanced by a factor of $10^3$.

REFERENCE:
COMMENT ON M2-E1 MIXING OBSERVED IN (\gamma,\gamma') REACTIONS

R. Moreh, A. Wolf and O. Shahal

It was shown that the effect of overlapping resonances in the photo-
excitation process of a (\gamma,\gamma') reaction is very small. The influence of this
effect on the angular distributions of the inelastic transitions and hence on
the M2/E1 mixing ratios was found to be negligible.

REFERENCE:

TOTAL RADIATIVE WIDTH OF BOUND NUCLEAR LEVELS EXCITED BY THE (\gamma,\gamma') REACTION

R. Moreh, A. Wolf, O. Shahal and J. Tenenbaum

The total radiative widths of bound nuclear levels, at an excitation
energy around 7 MeV, as a function of A were presented. These widths were
measured by employing self-absorption, temperature variation of the scattering
cross section and absolute cross section measurements. By comparing the present
results with the widths of unbound levels from (n,\gamma) work, it was shown that
the radiative widths are continuous across the (\gamma,n) threshold for these nuclei.

REFERENCE:
1. Moreh, R., Wolf, A., Shahal, O., and Tenenbaum, J., in: Int. Conf. on

ELASTIC AND RAMAN SCATTERING OF PHOTONS FROM $^{238}$U

T. Bar-Noy and R. Moreh

The results of measuring the elastic and Raman scattering cross sections
for 7 discrete photo energies between 7.9 and 11.4 MeV were given. It was
shown that by making slight changes in the parameters of the dipole resonance
of $^{238}$U, the measured scattering of the cross sections are found to be in fair
agreement with predictions of the simple rotator model.

REFERENCE:
1. Bar-Noy, T., and Moreh, R., in: Int. Conf. on Photonuclear Reactions and

DELBRUCK SCATTERING OF 7.9 MeV PHOTONS

R. Moreh and S. Kahane

The elastic scattering cross section of 7.9 MeV photons by U and Th
was measured in the angular range 25° - 140° . It was shown that at this
energy the forward elastic scattering is due almost entirely to Delbruck
scattering. The results are systematically lower by >50% than the calculated values. Good agreement with theory was obtained only after excluding the contribution of the real part of the Delbruck scattering amplitude.

REFERENCE:

AN AUTOMATIC COMPTON POLARIMETER FOR GAMMA ENERGIES IN THE RANGE 5-10 MeV

B. Arad and H. Szichman

A linear polarization analyzer based on a NaI Compton polarimeter and mini-computer was developed. Its use in photonuclear experiments and its reliability and advantages as compared with similar polarimeters were considered. Polarization measurements of the ground state transition from the 8.496 MeV level in $^{90}$Zr show that the transition is M1, indicating a positive parity for this level.

REFERENCE:

GAMMA DOSIMETER BASED ON USE OF A NE226 SCINTILLATOR

B. Divon, S. Eckhouse and M. Etzion

A gamma-radiation detector based on the use of a 2"x3" NE226 scintillator and a 56 AVP photomultiplier was tested as a dosimeter for relatively low γ dose rates in the presence of fast neutrons. The light output of the NE226 scintillator, as obtained for $^{60}$Co gamma rays, was measured to be about 30% of that of the NE102A scintillator having similar dimensions and light collection efficiency. The sensitivity of the detector was also measured as a function of the γ-ray energy. Relative sensitivities to gamma rays from $^{60}$Co, $^{137}$Cs, $^{22}$Na and the $^{19}$F($p$, $\gamma$)$^{16}$O reaction were found to be equal to the relative calculated energy absorption coefficients, within experimental error. As an example, the relative measured sensitivity of the NE226 scintillator to 1.25 MeV γ-rays from $^{60}$Co and 6.5 MeV γ-rays from $^{19}$F($p$, $\gamma$)$^{16}$O is 1.77, as compared with 1.71 for the NE102A scintillator.

The sensitivity to 14 MeV neutrons from the (D,T) reaction was also measured, and it was found that the relative sensitivity of the NE226 and NE102A scintillators is about 0.1. It was concluded that the relative sensitivity to 1.25 MeV γ-rays and 14 MeV neutrons of the NE226 dosimeter is about 1.5 : 1.
A WATER CERENKOV DETECTOR FOR THE DETECTION OF GAMMA RADIATION IN THE PRESENCE OF FAST NEUTRONS

S. Eckhouse, B. Divon and M. Shaanan

A water Cerenkov detector was evaluated as a gamma radiation detector having a low relative sensitivity to fast neutrons. Water was chosen as the medium due to its good transmission in the UV range. The photon production per unit volume and unit \( \gamma \) flux at energy \( E \), in a wavelength range \( \lambda_1 \) and \( \lambda_2 \) is:

\[
N(E) = A \left[ \frac{1}{\lambda_1} - \frac{1}{\lambda_2} \right] \int_{\lambda_{th}}^{T_{max}(E)} \frac{d\sigma(E, T)}{dT} I(\beta(T)) d\beta,
\]

where \( \frac{d\sigma(E, T)}{dT} \) is the Compton differential cross section for electron production at energy \( T \). \( T \) varies between the Cerenkov threshold and the Compton edge, and \( A \) is a constant. \( I(\beta(T)) \) is defined by:

\[
I(\beta(T)) = \int_{\beta_{th}}^{\beta(T)} (1 - \frac{1}{n^2 \beta^2}) \frac{\beta^3}{(1-\beta^2)^{3/2}} \left( \frac{dE}{dx} \right)^{-1} d\beta,
\]

where \( \beta_{th} \) is the value of \( \frac{\beta}{c} \) at the Cerenkov threshold, \( n \) is the index of refraction, and \( \frac{dE}{dx} \) is the stopping power of electrons in water.

Figure 1 illustrates the calculated results in the interval \( 2000\AA < \lambda < 7000\AA \). These results were verified experimentally by measuring the relative sensitivities at known gamma energies. The detector was constructed of a 2" diam by 6" high cylindrical container viewed by a 56 UVP photomultiplier. The sources used were \( ^{60}\text{Co} \), \( ^{24}\text{Na} \) and the \( ^{16}(p, \alpha)^{12} \) reaction at 3 MeV proton energy. The proton source was the Van de Graaff accellerator located at the Weizmann Institute. The measured relative sensitivities are summarized in Table 1.
The number of photons in the wavelength interval $2000 \AA \leq \lambda \leq 7000 \AA$ produced by a flux of $1 \gamma/cm^2$ in $1 \text{ cm}^3$ of water as a function of gamma energy.

**Fig. 1**

**TABLE 1**

Relative measured and calculated sensitivities

<table>
<thead>
<tr>
<th>Source</th>
<th>Energies (MeV)</th>
<th>Sensitivity per unit disintegration</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{60}\text{Co}$</td>
<td>$1.17$</td>
<td>measured: $1$, calculated: $1$</td>
</tr>
<tr>
<td></td>
<td>$1.33$</td>
<td></td>
</tr>
<tr>
<td>$^{24}\text{Na}$</td>
<td>$1.37$</td>
<td>measured: $2.38$, calculated: $2.26$</td>
</tr>
<tr>
<td></td>
<td>$2.75$</td>
<td></td>
</tr>
<tr>
<td>$^{16}\text{F(p,}\alpha)^{16}\text{O}$</td>
<td>$6$ $7$</td>
<td>measured: $5.8$, calculated: $5.46$</td>
</tr>
</tbody>
</table>
The sensitivity of the detector to neutrons was calculated taking into account the production of \( \gamma \)-rays by neutrons through reactions on \( ^{16}O \).

This sensitivity to 14 MeV neutrons was also measured using the \((D,T)\) reaction and found to be less by a factor of \( \sim 1.5 \) than the sensitivity to 1.25 MeV \( \gamma \)-rays from \( ^{60}Co \) whereas the calculated sensitivity differs by a factor of \( \sim 4 \). This discrepancy seems to be due to the reaction \( ^{16}O(n,p)^{16}N \), where the \( ^{16}N \) decays by \( \beta^- \) emission.

A SYSTEMATIC ODD-EVEN EFFECT IN THE INDEPENDENT YIELD DISTRIBUTIONS OF NUCLIDES FROM THERMAL NEUTRON FISSION OF \( ^{235}U \) (1)

S. Amiel and H. Feldstein

A detailed analysis of experimental fission yield data was found to exhibit a systematically consistent odd-even effect in the independent yield distributions of the nuclides in thermal neutron fission of \( ^{235}U \). The odd-even effect in the element yield distribution for elements at the fission peaks appears as a sawtooth structure, in which the amplitudes between the enhanced even-Z yields and the less favored odd-Z yields are \( \pm 2 \% \) of the mean values. The elements examined constitute 75\% of the fission yield.

The distribution of the isotopic yields in many cases was found to have a sawtooth pattern superimposed on a gaussian-like shape, where the amplitudes between the high even-N and low odd-N values are on the average \( \pm 8\% \) of the mean values. This effect seemed to be unresolved at the light peak nuclides while it was pronounced at the heavy peak nuclides.

The isobaric dispersions were studied in 24 mass chains (14 at the heavy mass peak and 10 at the light peak) and were found to follow the general pattern of a gaussian with widths varying between 0.45 and 0.8 charge units. The detailed description of the isobaric dispersion is represented by a sawtooth structure fluctuating with amplitudes of \( \leq 30\% \) around a constant width gaussian in which the even-Z nuclides are consistently enhanced. The only appearance of a significant closed shell effect is observed in \( ^{134}Te \).

The fact that the neutron pairing effect in the yields as compared with that of the protons is much smaller is attributed to the evaporation of neutrons during the de-excitation of the fragments, a process which is responsible for "washing out" of part of the original neutron pairing effect in the primary fragment formation in fission.
The experimental and "normal" (i.e., calculated by Wahl) independent yields of the elements formed in fission are presented in Table 2.

**TABLE 2**

Independent yields of complementary elements (Z, 92-Z) in thermal neutron fission of 235U

<table>
<thead>
<tr>
<th>Elements</th>
<th>Exp. yield, %</th>
<th>&quot;Normal&quot; yield, %</th>
<th>(Exp. yield - &quot;Normal&quot; yield) x 100* &quot;Normal&quot; yield</th>
</tr>
</thead>
<tbody>
<tr>
<td>As-Pr</td>
<td>1.2±0.1</td>
<td>1.4</td>
<td>-(14.3±7.1)</td>
</tr>
<tr>
<td>Se-Ce</td>
<td>4.3±0.3</td>
<td>3.6</td>
<td>+(19.4±8.3)</td>
</tr>
<tr>
<td>Br-La</td>
<td>5.9±0.4</td>
<td>7.6</td>
<td>-(22.4±5.3)</td>
</tr>
<tr>
<td>Kr-Ba</td>
<td>15.2±0.3</td>
<td>12.7</td>
<td>+(20.0±2.4)</td>
</tr>
<tr>
<td>Rb-Cs</td>
<td>11.7±0.5</td>
<td>15.1</td>
<td>-(22.5±3.3)</td>
</tr>
<tr>
<td>Sr-Xe</td>
<td>19.8±1.0</td>
<td>16.0</td>
<td>+(23.7±6.2)</td>
</tr>
<tr>
<td>Y-I</td>
<td>11.9±1.0</td>
<td>15.8</td>
<td>-(24.7±6.4)</td>
</tr>
<tr>
<td>Zr-Te</td>
<td>18.2±0.6</td>
<td>14.7</td>
<td>+(23.8±4.1)</td>
</tr>
<tr>
<td>Nb-Sb</td>
<td>9.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mo-Sn</td>
<td>2.9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Σ=88.2±1.4</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Average deviation from normal distribution ±(22.0±5.4)%

The present set of experimental data indicates the relative importance of the individual properties of the fragments versus the collective behavior of the fissioning nucleus, as described by the calculations of deformations of shell-corrected liquid drop potential energy surfaces. One is also led to conclude that nucleon transfer, apparent from the different charge densities of the fragments, takes place before scission and that at scission there is a smaller probability of breaking pair configurations, consistent with energy considerations.

**REFERENCE:**

STATUS OF DELAYED NEUTRON DATA

S. Amiel and T. Izak-Biran

The available delayed neutron data were reviewed. Since a few of the $P_n$ values were measured directly, we attempted to calculate $P_n$ values on the basis of experimentally measured delayed neutron yields and the recently determined fission yields. The contribution of the individual precursors to delayed neutron groups and total delayed neutron emission in thermal fission of $^{235}U$ was compared with experimental measurements. The fit seems satisfactory, but to obtain better accuracy the $P_n$ values will be recalculated based on newer values of thermal and fast fission yields for $^{235}U$ and $^{233}U$ to be determined shortly.

REFERENCES:

ON THE DETERMINATION OF FRACTIONAL FISSION YIELDS FROM THE CHEMICAL REACTION YIELDS IN THE GAS PHASE

Z.B. Alfassi and S. Amiel

The determination of fractional fission yields from the measured chemical yields of gaseous phase reaction products of fission fragments was studied in view of the kinetic theory of reactions of hot atoms. In order to have a linear dependence of the hot reactions yields on the reactant concentration it is suggested that reactants and moderators be used. These have a similar effect on the decrease of the energy of the hot atom ($\alpha_\gamma=\alpha_n$). For halogen atoms, it is suggested that methane be used as a reactant and not methyl halide.

REFERENCE:

ON-LINE STUDY OF GASEOUS FISSION PRODUCTS: RAPID TRANSFER TECHNIQUES

H. Feldstein and S. Amiel

The time required for a mass separated fission product to reach the collector may be considered to be composed of the time required to leave the fission source (by diffusion, emanation or recoil), the transfer time, and the

*Ben-Gurion University of the Negev, Beer-Sheva
mean residence time in the ion source. Since it is difficult to analyze each of these components separately, a number of transfer functions were derived for different configurations of target, transmission line and ion source, at different gas flow conditions, and the contribution of each stage to the overall delay was evaluated.

An adequate knowledge of the transfer time function is required for independent fission yield determinations in on-line mass separation studies, since the apparent yield of the separated fission product counted at the collector must be corrected for the decay occurring during the transfer from the irradiated target (especially in the case of short-lived isotopes) and for the decay of precursors in the target during irradiation and transfer.

REFERENCE:

A VERSATILE INTEGRATED TARGET-SURFACE IONIZATION SOURCE FOR ON-LINE ISOTOPE SEPARATIONS(1)

An integrated target-ion source designed to function both for negative and positive surface ionization was constructed. A large area target consisting of graphite foils coated with uranium is placed inside an heated chamber and exposed to a thermal neutron beam. The fission products diffuse out of the target chamber and pass through an heated tantalum guide tube, where they undergo ionization and are extracted into the mass separator (SOLIS). In the case of negative surface ionization, where halogens are separated, the intense electron emission is deflected by a small magnet placed near the exit of the ionization tube. The temperatures of the target and ionization chamber are controlled separately to optimize speed of separation, selectivity and ionization efficiencies. Diffusion time, efficiency and specificity as functions of the temperatures and dimensions were studied.

Collection and decay of activities were obtained for masses 92, 142 with positive surface ionization, and for masses 136-138 with negative surface ionization. The experimental surface ionization efficiencies were found in general agreement within a factor of 10 with the predicted values (e.g. 0.03% for I at $\sim$1400°C and $>$1% for Rb).
The specificity of separation was studied in detail for iodine. The contamination of iodine isotopes found to be $< 1:1000$ is due to the long diffusion time of tellurium (≈ 80 min at 1400°C) and its low ionization efficiency.

Independent fission yields of iodine isotopes of masses 135-139 were studied and further experiments dealing with nuclear spectroscopy and fission yield studies of alkalies and halogens from fission are in progress.

REFERENCE:
RADIATION CHEMISTRY AND APPLICATIONS
OF RADIATION AND RADIOISOTOPES
RADIATION-INDUCED DECHLORINATION OF CHLOROMETHANES - DETERMINATION OF ARRHENIUS PARAMETERS FOR CHLORINE ATOM ABSTRACTION BY CYCLOHEXYL RADICALS\(^1\)

M.G. Katz, A. Horowitz, G. Baruch and L.A. Rajbenbach

Gamma radiolysis of dilute solutions of chloromethanes (CM) in cyclohexane (RH) leads to a long chain dehalogenation process\(^2\) where RCl is one of the main products. In previous work we have shown\(^3\) that gamma irradiation of \(\text{C}_2\text{Cl}_4\) in RH results in a free radical chain substitution of a Cl atom by R. The irradiation of ternary solutions of \(\text{C}_2\text{Cl}_4\) and CM in RH gives rise to the occurrence of two different chain sequences in which RCl and R\(\text{C}_2\text{Cl}_3\) are formed. The Arrhenius parameters obtained from the kinetic analysis of the chain sequence are given in Table 1.

<table>
<thead>
<tr>
<th>CM</th>
<th>(\log A(\text{CM}) / \log A(\text{C}_2\text{Cl}_4))</th>
<th>(E(\text{CM}) - E(\text{C}_2\text{Cl}_4)) (kcal mole(^{-1}))</th>
<th>(\log A(\text{CM})) (&amp; mole(^{-1}) sec(^{-1}))</th>
<th>(E(\text{CM})) (kcal mole(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{C}_2\text{Cl}_4)</td>
<td>0.72±0.02</td>
<td>-1.42±0.05</td>
<td>9.40±0.08</td>
<td>5.88±0.11</td>
</tr>
<tr>
<td>(\text{CHCl}_3)</td>
<td>0.77±0.06</td>
<td>2.86±0.01</td>
<td>9.45±0.12</td>
<td>10.16±0.11</td>
</tr>
<tr>
<td>(\text{CH}_2\text{Cl}_2)</td>
<td>0.56±0.12</td>
<td>6.37±0.27</td>
<td>9.24±0.18</td>
<td>13.67±0.37</td>
</tr>
</tbody>
</table>

The possible application of the Evans-Polanyi relationship to the chlorine atom abstraction from CM was considered.

REFERENCES:

ABSTRACTION OF CHLORINE ATOMS FROM THE TRICHLOROMETHYL GROUP IN SEVERAL HALOETHANES. EFFECT OF NEIGHBORING GROUPS ON ARRHENIUS PARAMETERS

M.G. Katz, G. Baruch and L.A. Rajbenbach

The kinetics of halogen atom abstraction from haloethanes by the cyclohexyl radical was studied by a competitive technique.

The Arrhenius parameters for the abstraction of chlorine atoms from the following haloethanes were determined: \(\text{C}_2\text{Cl}_6\), \(\text{C}_3\text{Cl}_3\text{CCl}_3\text{H}\), \(\text{C}_3\text{Cl}_3\text{CH}_2\text{Cl}\), \(\text{C}_3\text{Cl}_3\text{CH}_3\) and \(\text{C}_3\text{Cl}_3\text{CF}_3\). The results obtained are given in Table 2.
TABLE 2
Arphenius parameters for Cl abstraction from the trichloromethyl group in haloethanes

<table>
<thead>
<tr>
<th>Haloethane</th>
<th>E(kcal mole(^{-1}))</th>
<th>log A (1 mole(^{-1}) sec(^{-1}))</th>
<th>Temperature range (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C(_3)C(_1)</td>
<td>5.02 ± 0.2</td>
<td>9.48 ± 0.11</td>
<td>22-190</td>
</tr>
<tr>
<td>C(_3)C(_2)H</td>
<td>6.10 ± 0.2</td>
<td>8.85 ± 0.11</td>
<td>40-200</td>
</tr>
<tr>
<td>C(_3)C(_3)H(_2)</td>
<td>8.15 ± 0.2</td>
<td>9.40 ± 0.10</td>
<td>100-220</td>
</tr>
<tr>
<td>C(_3)CH(_3)</td>
<td>9.35 ± 0.2</td>
<td>9.46 ± 0.11</td>
<td>100-225</td>
</tr>
<tr>
<td>C(_3)CF(_3)</td>
<td>6.14 ± 0.2</td>
<td>8.76 ± 0.11</td>
<td>60-200</td>
</tr>
</tbody>
</table>

It was shown that the neighboring group effect on the rate of chlorine atom abstraction from the trichloromethyl group can be correlated with Taft polar substituent constants.

CORRELATION OF ACTIVATION ENERGIES OF METATHETICAL FREE-RADICAL REACTIONS WITH POLAR, STERIC AND THERMOCHEMICAL PARAMETERS

M.G. Katz and L.A. Rajbenbach

Systematic studies of activation energies of the Cl atom abstraction from chloromethanes\(^{(1)}\) and chloroethanes\(^{(2)}\) by cyclohexyl radicals carried out in this laboratory enabled us to establish the fact that simple relationships between enthalpy and activation energy such as the Polanyi-Evans (P-E) equation, do not apply in this type of reaction. It can also be shown that the P-E equation does not apply in the case of H atom abstraction from chloroethanes by Cl atoms. The lack of a simple correlation between the enthalpies of reactions and the activation energies suggests that polar and possibly steric effects are of importance in the transition state of such reactions. In this study an effort was made to derive an expression for the activation energy which would contain quantitative corrective terms expressing the contribution of polar and steric effects.

For the reaction of a radical with a series of substituted molecules

\[ A + BC \rightarrow AC + B \]  \hspace{1cm} (1)

the following expression was derived,

\[ \Delta E_a = \alpha \Delta D + \rho \delta^* + \delta E_s \]  \hspace{1cm} (2)

where

\[ \Delta E_a \] the difference in the activation energies in the related series, where

B = CH\(_3\) serves as a reference reaction.
AD is the difference in bond association energies in the B-C series, where B = CH₃ serves as a reference reaction.

δ* is the Taft polar substituent constant.

Eₙ is the Taft steric substituent constant.

α, ρ, δ are appropriate coefficients characterizing the substrates and the radical.

A very good correlation between the experimental results for the reaction of the cyclohexyl radical with the series XCl₃ (where X denotes H, CH₃, CH₂Cl, etc.) and the derived expression (2) was obtained. The very low α factor derived (α = 0.02) indicates that the activation energy values for Cl atom abstraction are insensitive to thermochemical considerations. Equally good correlation was observed for H atom abstraction from the series XCH₃ and XC₂Cl₂H by Cl atoms. In this case α values of 0.30 and 0.25 were derived. These α values derived by us are in good agreement with those obtained by a different method for H atom abstraction by Cl atoms from hydrocarbons (3).

REFERENCES:

EFFECT OF PHASE ON THE ARRHENIUS PARAMETERS OF METATHETICAL RADICAL REACTIONS: Reaction of CC₃ Radicals with Cyclohexane

M.G. Katz and L.A. Rajbenbach

Dilute solutions of CC₃ in cyclohexane (RH) were irradiated and the RCl and C₂Cl₆ yields were determined. The formation of these products was considered in terms of the following reaction sequence:

\[ R + CC₃ \rightarrow RCl + CC₃ \]  
\[ CC₃ + RH \rightarrow CHCl₃ + R \]  
\[ R + R \rightarrow R₂ \]  
\[ R + CC₃ \rightarrow RCC₃ \]  
\[ CC₃ + CC₃ \rightarrow C₂Cl₆ \]

The rate constant ratio \( k₂/k₅ \) is given by

\[ k₂/k₅ = \frac{G(RCl)}{G(C₂Cl₆)} \cdot \frac{\alpha}{RH} \]

where \( \alpha \) is a constant that converts G values into rates of formation in units of mole \( \cdot \) sec⁻¹. The rate constant ratios \( k₂/k₅ \) were determined over a 30-110°C temperature range. The relative Arrhenius parameters obtained were:

\[ E₂ - \frac{E₅}{2} = 8.51 \pm 0.1 \text{ kcal mole} \text{ and } \log A₂/A₅ = 3.2 \pm 0.1. \]

Substituting the known
value $2k_5 = 10^8 \text{ M}^{-1} \text{ sec}^{-1}$ and assuming that the $E_5$ value is equal to the diffusion activation energy (4.54 kcal mole$^{-1}$), we obtained log $A_5 = 10.7$. From the relative rate expression we obtained $E_2 = 10.7$ kcal mole$^{-1}$ and $A_2 = 8.55$. These values are in good agreement with the gas phase determination. We thus conclude that meta-
thetical reactions in inert solvents are not affected by phase effects.

GAMMA RADIATION-INDUCED FORMATION OF ALKYL SULFONYL RADICALS IN CYCLOHEXANE
A. Horowitz and L.A. Rajbenbach

The radiolysis of alkylsulfonyl chlorides (RSO$_2$Cl, where $R = \text{Me, n-Pr or n-Bu}$) was studied over the temperature range 23°-200°C. It was found that the alkylsulfonyl chlorides are decomposed by a free-radical chain mechanism. The propagation steps of this chain are:

$$\text{RSO}_2\text{Cl} + \text{c-C}_6\text{H}_{11} \rightarrow \text{RSO}_2 + \text{c-C}_6\text{H}_{11}\text{Cl} \quad (1)$$

$$\text{RSO}_2 + \text{c-C}_6\text{H}_{11} \rightarrow \text{RSO}_2\text{H} + \text{c-C}_6\text{H}_{11} \quad (2)$$

By kinetic analysis $k_2$ values were estimated from the rates of chlorocyclohexane formation. In ternary solutions that contained tetrachloroethylene, reaction (1) competes with reaction (3).

$$\text{c-C}_6\text{H}_{11} + \text{C}_2\text{Cl}_4 \rightarrow \text{c-C}_6\text{H}_{11}\text{Cl} + \text{C}_2\text{Cl}_3 + \text{Cl} \quad (3)$$

The rate constant ratio $k_1/k_3$ was determined in this system.

THE EFFECT OF SUBSTITUTION BY CN ON THE Reactivity OF CHLOROALKANES
Y. Gonen, A. Horowitz and L.A. Rajbenbach

The effect of substitution by the cyano group on the reactivity of chloroalkanes in chlorine transfer reactions was studied on a model system, namely trichloroacetonitril in cyclohexane (RH). The thermally and radiolytically induced decomposition of CCl$_3$CN solutions was found to lead to the formation of HCCl$_2$ and RCl by a free radical chain mechanism. The rate constants $k_1$ and $k_2$ and the respective Arrhenius parameters of the chain propagation steps (1) and (2) were determined.

$$\text{R} + \text{CCl}_3\text{CN} \rightarrow \text{c-C}_6\text{H}_{11}\text{Cl} + \text{CCl}_2\text{CN} \quad (1)$$

$$\text{CCl}_2\text{CN} + \text{RH} \rightarrow \text{HCCl}_2\text{CN} + \text{R} \quad (2)$$

Comparisons of the findings of this work with the results obtained for the analogous reactions in the CCl$_4$ - RH system indicates that the substitution of a chlorine atom by a cyano group results in the lowering of the activation energy for chlorine transfer by about 4 kcal/mole. This difference probably reflects the stabilization effect of the CN group in the CCl$_2$CN radical. Indeed, according to our results CCl$_2$CN requires an activation energy for hydrogen abstraction from
cyclohexane which is higher by about 4 kcal than the activation energy for the abstraction of hydrogen by CCl₃.

EFFECT OF F ATOMS ON THE STABILITY OF BROMO-METHYL RADICALS
M. Ben-Yehuda and L.A. Rajbenbach

The effect of fluorine substitution on the ease of abstraction of bromine atoms from halomethanes by cyclohexyl radicals was studied over an extended temperature range. Radiolytic initiation of the free-radical chain dehalogenation sequence was employed. The kinetic scheme can be represented as follows:

\[ 2RH \rightarrow 2R + H_2 \]  \hspace{1cm} (1)

\[ R + C_{XBr\text{-}n} \rightarrow RBr + CXBr_{\text{-}(n+1)} \]  \hspace{1cm} (2)

\[ R + C_2Cl_4 \rightarrow RC_2Cl_4 \rightarrow RC_2Cl_3 + Cl \]  \hspace{1cm} (3)

The bromine atom abstraction reaction data can be put on an absolute basis by comparing the rates of metathesis (reaction 2) with the known rate of addition of R radicals to C₂Cl₄ (reaction 3). Preliminary results indicate that fluorine substitution significantly reduces the activation energy of the metathetical step, (reaction 2).

REFERENCE:

GAMMA-RADIATION-INDUCED OXIDATION OF METHANOL BY HEXACHLOROETHANE
R. Aloni, L.A. Rajbenbach and A. Horowitz

The radiolysis of hexachloroethane solutions in methanol was studied over the temperature range 26°C-100°C. Typical results of the radiolysis of a 0.1M solution of C₂Cl₆ are shown in Table 3. It can be seen that hexachloroethane is consumed with high G values at relatively moderate temperatures.

**TABLE 3**

<table>
<thead>
<tr>
<th>Temp. (°C)</th>
<th>Total dose (eV ml⁻¹ x 10⁻¹⁶)</th>
<th>G(C₂Cl₄)</th>
<th>G(C₂Cl₅H)</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>24.6</td>
<td>985</td>
<td>455</td>
</tr>
<tr>
<td>50</td>
<td>29.5</td>
<td>95</td>
<td>390</td>
</tr>
<tr>
<td>76</td>
<td>9.8</td>
<td>7777</td>
<td>769</td>
</tr>
<tr>
<td>93</td>
<td>4.9</td>
<td>7648</td>
<td>830</td>
</tr>
<tr>
<td>100</td>
<td>9.8</td>
<td>11160</td>
<td>998</td>
</tr>
</tbody>
</table>
The free radical mechanism that accounts for the observed high conversion yields is given by the following reaction sequence:

**Initiation (schematic)**

\[
2\text{CH}_3\text{OH} \rightleftharpoons 2\text{CH}_2\text{OH} + \text{H}_2
\]

**Propagation**

\[\text{CH}_2\text{OH} + \text{C}_2\text{Cl}_6 \rightarrow \text{CICH}_2\text{OH} + \text{C}_2\text{Cl}_5 \quad (1)\]
\[\text{CICH}_2\text{OH} \rightarrow \text{CH}_2\text{O} + \text{HCl} \]
\[\text{C}_2\text{Cl}_5 \rightarrow \text{C}_2\text{Cl}_4 + \text{Cl} \quad (2)\]
\[\text{C}_2\text{Cl}_5 + \text{CH}_2\text{OH} \rightarrow \text{C}_2\text{Cl}_4\text{H} + \text{CH}_2\text{OH} \quad (3)\]
\[\text{Cl} + \text{CH}_2\text{OH} \rightarrow \text{HCl} + \text{CH}_2\text{OH} \quad (4)\]

**Termination**

Various biradical reactions

This mechanism was verified by the good balance between \(G(\text{C}_2\text{Cl}_6)\) and \(G(\text{Cl}_2\text{H}) + G(\text{C}_2\text{Cl}_4)\).

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ON THE MECHANISM OF REDUCTION OF PORPHYRINS. A PULSE RADIOLYTIC STUDY\(^1\)

Y. Harel and D. Meyerstein

The mechanisms of reduction of haematoporphyrin, \(\text{PH}_2\), and its Zn complex, \(\text{ZnP}\), by strong single electron reducing agents in alkaline aqueous solution were studied. It was found that for both compounds three intermediates are formed prior to the formation of the stable products. The mechanism of reduction of both compounds seems to be the following:

a) \(\text{PH}_2/\text{ZnP} + \text{R}^- \rightarrow k_1 \quad \text{PH}_3^- \text{ or } (\text{PH}_3^-)/(\text{ZnP})\text{(ZnP}^-) + \text{R}^-\text{,where } k_1\text{ depends on }\text{R}^-.\]

\[k_2 = 2.1 \times 10^8 \text{ M}^{-1} \text{sec}^{-1}\]

b) \(2\text{PH}_3/2\text{ZnP}^- \rightarrow (\text{PH}_3)_2/(\text{ZnP})_2\)

where the dimer is plausibly a \(\pi\)-mer.

\[k_{\text{PH}_2} = 10 \text{ sec}^{-1}\]

\[k_{\text{ZnP}} = 17 \text{ sec}^{-1}\]

This reaction seems to be some kind of rearrangement of the dimer.

d) In this step the mechanisms differ

\[(\text{PH}_3)_2\longrightarrow k = 0.11 \text{ sec}^{-1} \rightarrow \text{PH}_4 \text{ or } (\text{PH}_3^+) + \text{PH}_2\]

\[(\text{ZnP})_2\longrightarrow \text{Zn (dihydroporphyrin) + ZnP}\]

where \(\text{PH}_4\) is a phlorin, whereas in the Zn (dihydroporphyrin) one of the hydrogen atoms is added on a peripheral position.

This mechanism is nearly independent of \(\text{pH}\) in the \(7<\text{pH}<13\) range and of the solvent water, methanol or ethanol. The absorption spectra of all intermediates
were reported.

The reduction of haemin by $e^{-}$ or CH$_3$CHO$^-$ on the other hand proceeds via direct reduction of the central Fe(III) to Fe(II) in one step.

REFERENCE:

KINETICS OF REACTION OF FERRICENIUM ION WITH SOME FREE RADICALS IN AQUEOUS SOLUTION. A PULSE RADIOLYTIC STUDY.
Z. Teitelbaum and D. Meyerstein

Several authors have suggested that ferricenium ion is an active intermediate in some free radical and electrophilic substitution reactions of ferrocene$^{(1,2)}$. Following these reports we attempted to study the mechanism of reaction of ferricenium ion with several free radicals, in aqueous solutions, using the pulse radiolysis technique.

The results indicate that radicals which are powerful single electron reducing agents (e.g. H atoms, -CH$_2$OH, CH$_3$CHOH and (CH$_3$)$_2$COH), reduce ferricenium to yield ferrocene. The specific rate constants of these reactions approach the diffusion controlled limit. No intermediates were observed in these reactions. The rate of reaction of the ferrocene, formed in these reactions, with Fe$^{+3}_{aq}$ present in the solution is in fair agreement with the value reported in the literature$^{(3)}$.

Non-reducing radicals, such as those derived from acetic acid, propionic acid and tert-butanol, react with ferricenium with lower rate constants, by two to three orders of magnitude, than those of the reducing radicals.

It was found that even oxidizing radicals, like OH, Br$_2^-$ and Cl$_2^-$ radicals, react with ferricenium in aqueous solution. These reactions occur by a more complex mechanism than those with reducing radicals. Thus for example, Br$_2^-$ reacts with ferricinium with a specific rate constant of $3\times10^8$ M$^{-1}$sec$^{-1}$. This reaction is followed by at least two further steps until stable products are formed. A major stable product is a substituted ferrocene, which is not oxidized by Fe$^{+3}_{aq}$. The mechanism of these reactions and the nature of the intermediates were considered.

REFERENCES:
CHROMIUM-CARBON BONDS IN AQUEOUS SOLUTIONS. A PULSE RADIOLYTIC STUDY(1)
H. Cohen and D. Meyerstein

The specific rates of reaction of sixteen aliphatic radicals with Cr(H_2O)_6^{2+} were determined. The absorption spectra due to the chromium-carbon bonds in the products of these reactions were measured. The specific rates of reaction of these complexes as a function of pH were determined. The effects of the structure of the aliphatic radicals on these spectra and specific rates of reactions were considered in detail. It was shown that chromium induces water elimination when a $\text{S}$-hydroxyl group is present.

REFERENCE:

ON THE SPECTRA, KINETICS OF FORMATION AND DECOMPOSITION OF PENTA-AQUO-CHROMIUM(III) HYDRIDE AND AQUO CHROMIUM(I) IN AQUEOUS SOLUTIONS. A PULSE RADIOLYTIC STUDY(1)
H. Cohen and D. Meyerstein

The reaction of hydrogen atoms with Cr^{2+}_{aq} was studied:

$$k_{\text{Cr}^{2+}_{aq}+H} = 1.5 \times 10^{9} \text{ M}^{-1} \text{ sec}^{-1}.$$ The product of this reaction was identified as Cr(H_2O)_5^{2+}. The absorption spectrum of this compound was measured and found to be similar to that of compounds containing chromium-carbon bonds. The mechanism of decomposition of Cr(H_2O)_5^{2+} obeys the rate law $k_1 + k_2 [H_3O^+]$ where $k_2 = 1.8 \times 10^4 \text{ M}^{-1} \text{ sec}^{-1}$ and $k_1 < 1 \text{ sec}^{-1}$. In neutral solutions Cr^{2+}_{aq} is formed by the reaction of $e^{-}_{aq}$ with Cr^{2+}_{aq}. The absorption spectrum of Cr^{2+}_{aq} and the kinetics of its decomposition were considered together with the implication of the results on the mechanism of dissociation of chromium metal and on the photochemistry of Cr^{2+}_{aq}.

REFERENCE:

THE HOT DISPLACEMENT REACTIONS OF $^{38}\text{Cl}$ WITH CH$_3$Br AND $^{80}\text{Br}$ WITH CH$_3$Cl IN THE GAS PHASE. EVIDENCE FOR A POSSIBLE BILLIARD BALL MECHANISM(1)
Z.B. Alfassi* and S. Amiel

The yields of the various products of the reactions of hot $^{38}\text{Cl}$ with CH$_3$Br and hot $^{80}\text{Br}$ with CH$_3$Cl were measured for different concentrations of noble gas moderator (He for the first reaction and Ne for the second). The reactivity integrals and the average logarithmic energy losses of the hot atoms colliding with the reactant molecules were calculated. Average logarithmic energy decrement values of 5.6 $\alpha_{\text{Cl-He}}$ and 3.2 $\alpha_{\text{Br-Ne}}$, and the reactivity integrals 0.24 $\alpha_{\text{Cl-He}}$ and

*Ben-Gurion University of the Negev, Beer Sheva
0.097 $^3$Br-Ne were derived. Comparison of the above reactions with each other and with the reactions of $^{38}$Cl with CH$_2$Cl and $^{80}$Br with CH$_2$Br suggest that a billiard ball mechanism may be responsible to a considerable extent for all four reactions.

REFERENCE:

THE REACTION OF HOT $^{38}$Cl AND $^{80}$Br WITH CH$_2$ClBr. ANOTHER EXAMPLE OF THE "TRANSLATIONAL INERTIAL EFFECT"(1)
Z.B. Alfassi* and S. Amiel

The yields of the different products of the reactions of $(n,\gamma)$ produced hot $^{38}$Cl and hot $^{80}$Br atoms with CH$_2$ClBr were studied in order to find the relative importance of the billiard ball model and the translational inertial effect. The experimental results, given in Table 4, show that in the reaction of hot chlorine atoms with CH$_2$ClBr there is a preferable displacement of a bromine atom over a chlorine atom. This is in accordance with the "translational inertial effect", indicating that this may be the main mechanism determining the displacement.

TABLE 4
Yields of the displacement reactions of hot $^{38}$Cl and $^{80}$Br with CH$_2$ClBr

<table>
<thead>
<tr>
<th>System</th>
<th>Displacement of a bromine atom</th>
<th>Displacement of a chlorine atom</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{80}$Br + CH$_2$ClBr</td>
<td>0.28%</td>
<td>0.15%</td>
</tr>
<tr>
<td>$^{38}$Cl + CH$_2$ClBr</td>
<td>1.95%</td>
<td>0.25%</td>
</tr>
</tbody>
</table>

REFERENCE:

THE PHOTODISSOCIATION OF IODOAROMATICs IN SOLUTION(1)
A. Levy, D. Meyerstein and M. Ottolenghi**

Deiodination and isotopic-exchange processes were employed for determining the photodissociation yields of various iodoaromatic molecules in solution as a function of temperature and excitation wavelength. In the case of 1-iodonaphthalene the direct-excitation yields were compared with those obtained by photosensitization with benzophenone. The data indicate that dissociation takes place after thermal relaxation from either singlet or lowest triplet states. Photodissociation of these two excited states exhibits a different temperature dependence. Rate constants for the reaction of phenyl radicals with aromatic scavengers were determined and

*Ben-Gurion University of the Negev, Beer Sheva

**Hebrew University, Jerusalem
considered along with the possibility of H-atom migration within the radical ring.

REFERENCE:

ON THE KINETIC TREATMENT OF PHOTOCHEMICALLY-INDUCED ISOTOPIC EXCHANGE
A. Levy, D. Meyerstein and M. Ottolenghi

A kinetic treatment describing the time dependence of the exchanged fraction (F) was presented for the photochemically-induced isotopic exchange process:

\[ AX + BX \xrightarrow{hv} AX^* + BX \]

when complicated by a net change in the concentration of AX due to the side reaction:

\[ AX \xrightarrow{hv} BX \]

The kinetic equations were numerically integrated and applied to the specific case in which \( AX = \) iodobenzene and \( BX = \) radioactive iodine (\( ^{131}\)I). The treatment accounts quantitatively for the experimental F vs. time plots. It also leads to the evaluation of the relative rate constants of the phenyl radical (Ph-) scavenging processes:

\[ \text{Ph}^- + I_2 \rightarrow \text{PhI} + I^- \]

and

\[ \text{Ph}^- + S \rightarrow \text{scavenging products} \]

where S is benzene, toluene or molecular oxygen.

REFERENCE:

THE PHOTOCHEMICAL REACTION OF Cd WITH CH\(_3\)Cl
M. Freiberg, S. Weiss and D. Meyerstein

The reaction of Cd vapor, irradiated with an isotopic Cd lamp, with CH\(_3\)Cl was investigated at 250°C. No isotopic enrichment could be discovered in the CdCl\(_2\) produced. The lack of enrichment is attributed to an isotopic exchange reaction. The results are given in Table 5.

REFERENCE:
<table>
<thead>
<tr>
<th>No.</th>
<th>Reactants</th>
<th>Lamp</th>
<th>Temperature, °C</th>
<th>Product</th>
<th>Isotopic comp. of product</th>
<th>Irrad. time (h)</th>
<th>Flow rate mmol/sec</th>
<th>Product yield mg</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CH₃Cl+Cd</td>
<td>nCd</td>
<td>Uncooled (440)</td>
<td>CdCl₂</td>
<td>-</td>
<td>15</td>
<td>0.4</td>
<td>1.0-2.5</td>
<td>Several expts., similar cond.</td>
</tr>
<tr>
<td>2</td>
<td>CH₃Cl+Cd</td>
<td>-</td>
<td>300</td>
<td>CdCl₂</td>
<td>-</td>
<td>20</td>
<td>0.4</td>
<td>0.05</td>
<td>Thermal blank, several expts.</td>
</tr>
<tr>
<td>3</td>
<td>CH₃Cl+Cd</td>
<td>-</td>
<td>400</td>
<td>CdCl₂</td>
<td>-</td>
<td>15</td>
<td>0.6</td>
<td>0.01</td>
<td>Thermal blank</td>
</tr>
<tr>
<td>4</td>
<td>CH₃Cl+Cd</td>
<td>-</td>
<td>300</td>
<td>CdCl₂</td>
<td>-</td>
<td>15</td>
<td>0.6</td>
<td>0.05</td>
<td>Thermal + microwave generator blank</td>
</tr>
<tr>
<td>5</td>
<td>CH₃Cl+Cd</td>
<td>nCd</td>
<td>440</td>
<td>CdCl₂</td>
<td>-</td>
<td>15</td>
<td>0.5</td>
<td>0.4-0.6</td>
<td>Several expts. with 1-4 Pyrex filters 1 mm thickness</td>
</tr>
<tr>
<td>6</td>
<td>CH₃Cl+Cd</td>
<td>nZn</td>
<td>300</td>
<td>CdCl₂</td>
<td>-</td>
<td>20</td>
<td>0.5</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>CH₃Cl+Cd</td>
<td>110Cd</td>
<td>440</td>
<td>CdCl₂</td>
<td>NA*</td>
<td>20</td>
<td>0.6</td>
<td>1.3</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>CH₃Cl+Cd</td>
<td>110Cd</td>
<td>300</td>
<td>CdCl₂</td>
<td>NA*</td>
<td>27</td>
<td>0.6</td>
<td>1.4</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>CH₃Cl+Cd</td>
<td>106Cd</td>
<td>440</td>
<td>CdCl₂</td>
<td>NA*</td>
<td>21</td>
<td>0.5</td>
<td></td>
<td>Several expts.</td>
</tr>
<tr>
<td>10</td>
<td>CH₃Cl+Cd</td>
<td>106Cd</td>
<td>130</td>
<td>CdCl₂</td>
<td>NA*</td>
<td>3.5-14</td>
<td>0.5</td>
<td>0.8-2.5</td>
<td>Several expts.</td>
</tr>
<tr>
<td>11</td>
<td>CH₃Cl+Cd+Hg</td>
<td>106Cd</td>
<td>150-200</td>
<td>CdCl₂</td>
<td>NA*</td>
<td>8</td>
<td>0.4</td>
<td>4.8</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>CH₃Cl+Cd+Hg</td>
<td>-</td>
<td>300</td>
<td>CdCl₂</td>
<td>-</td>
<td>10</td>
<td>0.4</td>
<td>0.04</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>CH₃Cl+Cd+Hg</td>
<td>nHg</td>
<td>150</td>
<td>CdCl₂</td>
<td>-</td>
<td>7</td>
<td>0.6</td>
<td>1.85</td>
<td>Hole fraction CdCl₂/HgCl₂ = 10</td>
</tr>
<tr>
<td>14</td>
<td>CH₃Cl(80%) +Ethylene(20%) +Cd</td>
<td>106Cd</td>
<td>150-200</td>
<td>CdCl₂</td>
<td>NA*</td>
<td>12</td>
<td>0.4</td>
<td>4.8</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>CH₃Cl+Cd</td>
<td>106Cd</td>
<td>Pyrex filter</td>
<td>CdCl₂</td>
<td>NA*</td>
<td>9</td>
<td>0.4</td>
<td>1.4</td>
<td></td>
</tr>
</tbody>
</table>

* NA = Natural abundance
INDUSTRIAL APPLICATIONS OF IONIZING RADIATION

The applied research being directed toward the modification of the properties of plastic materials by radiation technology and to the radiation curing of polymeric substances was continued under the sponsorship of industry and the National Council for R&D. The radiation facilities used comprised an industrial 550 keV electron accelerator and $^{60}$Co sources.

1. CROSSLINKING OF POLYMERS BY RADIATION (J. Wallach, G. Waldner and L.A. Rajbenbach)

The conditions of radiation cross linking of several polymers were optimized. Multifunctional monomers as well as low molecular weight polymers containing unsaturated bonds were incorporated into the substrates prior to irradiation.

2. MODIFICATION OF PERMEABILITY PROPERTIES OF PLASTIC FILMS (S. Amdur, L.A. Rajbenbach and G. Waldner)

Radiation grafting of mixtures of suitable monomers onto the surface of the substrates was continued. Emphasis was on the achievement of a homogeneous film deposition on the treated surface.

3. IMPARTING OF FIRE RETARDATION PROPERTIES TO POLYMERS (S. Amdur, G. Waldner and L.A. Rajbenbach)

The efficacy of mixtures of bromine- and chlorine-bearing organic compounds as fire retarding agents was studied. The influence of several phosphor-bearing additives on the fire retarding properties of the halogenated agents was evaluated. Different modes of incorporation of the fire-retarding agents were tried and the relative advantages of these methods were evaluated.

4. CURING OF PREPOLYMERS BY RADIATION (A. Mei-Marom and G. Waldner)

This project was continued with emphasis on perfecting the composition of the prepolymer mixture used in coating processes. Optimal radiation intensity and dose levels were also evaluated.

PRELIMINARY EXPERIMENTS ON THE INFLUENCE OF ELECTRONS AND GAMMA IRRADIATION ON THE EXTERNAL APPEARANCE OF VALENCIA ORANGES

R. Padova

Valencia oranges of export quality, which were picked in the middle of March and the end of May, were irradiated with doses of 25, 50 and 100 krads of electrons or gamma rays. Before irradiation, each dose batch
was either waxed, or waxed and packaged in polyethylene bags. These fruit were compared with unwaxed oranges. After irradiation the fruit was stored at 13°C and 90% relative humidity.

The fruits were checked after one month for external appearance, ranked as sort A, B or unsalable, and also for percent rots. The results show that after gamma irradiation unwaxed oranges were 70-100% unsalable, whereas waxed oranges showed a higher rate of salable fruit: 95% after 25 krad and 75% after 100 krad doses.

In contrast, after electron irradiation in all cases the rate of salable fruit was higher than after gamma irradiation at the same doses and reached 95-100%, even after receiving 100 krads, waxing and packaging in polyethylene. The percent of rots was generally low, although higher in unwaxed fruit.

### PRODUCTION OF TRITIUM AND CARBON-14 LABELLED COMPOUNDS


The production of tritium and carbon-14 labelled molecules was continued with emphasis mainly on those items which have a regular market. In addition to the compounds described previously, some new derivates were labelled. A detailed list is given in Table 6. The specific activities refer to chemically and radiochemically pure compounds.

#### TABLE 6 - New labelled compounds

<table>
<thead>
<tr>
<th>Precursor</th>
<th>Compound</th>
<th>Type of labelling</th>
<th>Spec. Activity Ci/mmole</th>
</tr>
</thead>
<tbody>
<tr>
<td>fluorobenzene</td>
<td>1-fluoro-2,4-dinitro-3,5,6-T (D.N.F.B.)</td>
<td>Specific (5)</td>
<td>6.76</td>
</tr>
<tr>
<td>5-hydroxymethyl-4-methyl-thiazole</td>
<td>5-hydroxymethyl-4-methyl-thiazole-T</td>
<td>General (6)</td>
<td>0.217</td>
</tr>
<tr>
<td>oleic acid</td>
<td>stearic acid-9, 10-T</td>
<td>Specific (7)</td>
<td>27.2</td>
</tr>
<tr>
<td>palmitoleic acid</td>
<td>palmitic acid-9,10-T</td>
<td>Specific (7)</td>
<td>25.8</td>
</tr>
<tr>
<td>L-lysine.HCl</td>
<td>L-lysine-T</td>
<td>General</td>
<td>0.067</td>
</tr>
<tr>
<td>N-methyl-4-piperidyl-benzilate</td>
<td>N-methyl-4-piperidyl-benzilate-T</td>
<td>General</td>
<td>6.3</td>
</tr>
<tr>
<td>6-chloro uracil</td>
<td>uracil-5,6-T</td>
<td>Specific (8)</td>
<td>39.0</td>
</tr>
<tr>
<td>ethacrynic acid</td>
<td>ethacrynic acid-T</td>
<td>General</td>
<td>3.34</td>
</tr>
<tr>
<td>benzoic acid</td>
<td>benzoic acid-T</td>
<td>General</td>
<td>0.068</td>
</tr>
<tr>
<td>benzophenone</td>
<td>benzo phenone-T</td>
<td>General</td>
<td>0.354</td>
</tr>
<tr>
<td>bibenzyl</td>
<td>bibenzyl-T</td>
<td>General (9-11)</td>
<td>0.341</td>
</tr>
<tr>
<td>thymine-2-C-14</td>
<td>thymidine-2-C-14</td>
<td>Specific</td>
<td>0.060</td>
</tr>
</tbody>
</table>
REFERENCES:
8. Pfleiderer, W. and Deiss, H., Israel J. Chem. 6, 603 (1968)
PHYSICAL AND INORGANIC CHEMISTRY
INTERACTIONS IN AQUEOUS TERNARY SYSTEMS
D. Rosenzweig and J. Padova

Activity coefficients of Me$_4$NBr and Pr$_4$NBr dissolved in NaBr aqueous solutions\(^{(1)}\) were calculated and the results are presented in Figs. 1 and 2. Figure 3 represents the excess free energy of mixing for the system Me$_4$NBr-NaBr-H$_2$O. From these results and others given elsewhere\(^{(2)}\), the following conclusions may be drawn.

![Fig. 1](image1.png)
Regional activity coefficients of Me$_4$NBr in the Me$_4$NBr-NaBr system

![Fig. 2](image2.png)
Regional activity coefficients in the Pr$_4$NBr-NaBr system
Free energy of mixing in the Me₄NBr-NaBr-H₂O system

Me₄NBr-NaBr system: Curves of excess free energy of mixing ($\Delta_{m}^{G^{EX}}$) vs rational mole fraction of Me₄NBr ($y_{e}$) start with positive values at low concentrations and go to negative values at high concentrations. The curves at high concentrations are nearly symmetric. These facts indicate that the Me₄N⁺ ion tends to create a Me₄N⁺-Me₄N⁺ interaction at low concentrations, but this tendency is compensated for by the effect of the ion-pair formation of Me₄N⁺-Br⁻. A Na⁺ ion attaches itself to this ion-pair to form a new triplet Me₄N⁺-Br⁻-Na⁺. The ion-pair and the triplet tend to break the water structure, and this phenomenon results in the "salting-out" of the Me₄NBr.

Pr₄NBr-NaBr system: In this system the $\Delta_{m}^{G^{EX}}$ values are positive for all concentrations and mole fractions, but the maximum height of the curves of $\Delta_{m}^{G^{EX}}$ vs $y_{e}$ is shifted towards the NaBr direction. It is concluded that the hydrophobic interaction, Pr₄N⁺-Pr₄N⁺ is very strong at low concentrations.
At high concentrations it was possible to detect fifth order interactions. The organic ion predominates in the interactions and may be considered to form micelles in the system. At high total concentrations and high rational mole fractions of Pr₂NBr the high order interactions cause "salting-in" of the Pr₂NBr.

REFERENCES:

MULTICOMPONENT SYSTEMS IN AQUEOUS SOLUTIONS*
D. Saad and J. Padova

As a part of a general isopiestic study of polycomponent electrolyte solutions, the quaternary system KCl-NaCl-MgCl₂-H₂O was investigated at 25°C at a constant ratio

\[ \frac{m_{KCl}}{m_{NaCl}} = 1.33 \]

The apparatus and procedure have been described previously(1). Equilibrium isopiestic-ionic strengths of solutions are presented in Table 1.

**TABLE 1**
Isopiestic-ionic strength at equilibrium

<table>
<thead>
<tr>
<th>( y_1 )</th>
<th>Set No.</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>2.268</td>
<td>1.756</td>
<td>1.686</td>
<td>0.934</td>
<td>0.596</td>
<td></td>
</tr>
<tr>
<td>0.1393</td>
<td>2.392</td>
<td>1.863</td>
<td>1.790</td>
<td>0.996</td>
<td>0.639</td>
<td></td>
</tr>
<tr>
<td>0.2836</td>
<td>2.545</td>
<td>1.997</td>
<td>1.916</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>0.4399</td>
<td>2.722</td>
<td>-</td>
<td>-</td>
<td>1.179</td>
<td>0.762</td>
<td></td>
</tr>
<tr>
<td>0.5994</td>
<td>-</td>
<td>2.329</td>
<td>2.244</td>
<td>1.296</td>
<td>0.847</td>
<td></td>
</tr>
<tr>
<td>0.7350</td>
<td>3.139</td>
<td>2.509</td>
<td>2.422</td>
<td>1.419</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>0.8678</td>
<td>3.357</td>
<td>-</td>
<td>2.622</td>
<td>1.576</td>
<td>1.048</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>3.601</td>
<td>2.950</td>
<td>2.853</td>
<td>1.745</td>
<td>1.178</td>
<td></td>
</tr>
</tbody>
</table>

\[ y_1 = \frac{3m_1}{I}; \quad I = 3m_1 + m_2 + m_3 \]

\( m_1, m_2, m_3 \) are the molalities of MgCl₂, NaCl and KCl, respectively.

Osmotic coefficients, activity coefficients of MgCl₂, Harned's and Friedman's coefficients and excess Gibbs free energies of mixing were calculated(2). The experimental data were treated by modifications of the

* This work is partly supported by the Ministry of Development
Scatchard\(^{(3)}\) and McKay-Perring\(^{(4)}\) equations, and good agreement between the two methods (difference of 0.010 or less in log \(Y_{\text{trace}}\) of the MgCl\(_2\)) was obtained. The calculations indicate a low probability of getting cation-cation interactions \(\text{Mg}^{++-\text{K}^+}, \text{Mg}^{++-\text{Na}^+}\) by mixing KCl-NaCl-H\(_2\)O solutions with MgCl\(_2\) solutions. This may be seen in Fig. 4, where \(g_0\) (first Friedman coefficient) is plotted against the ionic strength. Positive values of \(g_0\) point to a low probability of new interactions due to mixing. The probability of \(\text{Mg}^{++-\text{K}^+}, \text{Mg}^{++-\text{Na}^+}\) interactions in the quaternary system is lower than in the ternary systems MgCl\(_2\)-KCl-H\(_2\)O and MgCl\(_2\)-NaCl-H\(_2\)O due to the strong cation-cation interaction \(\text{K}^+-\text{Na}^+\) in the pseudo-binary solutions of KCl-NaCl-H\(_2\)O before mixing with the magnesium chloride solutions.

Fig. 4
Comparison of the first Friedman coefficient \(g_0\) as a function of ionic strength for several systems

REFERENCES:
DETERMINATION OF ACTIVITY COEFFICIENTS IN AQUEOUS MIXTURES OF \( \text{LiBr-MgBr}_2\cdot\text{H}_2\text{O} \), \( \text{NaBr-MgBr}_2\cdot\text{H}_2\text{O} \) and \( \text{KBr-MgBr}_2\cdot\text{H}_2\text{O} \)

J. Padova and J. Auslaender

The activity coefficients of alkali bromides in aqueous solution of magnesium bromide were determined at 25°C using a cation selective electrode. The method and procedure have already been described\(^{(1)}\). The activity of magnesium bromide was obtained by a Gibbs-Duhem transform and results obtained for all systems seem to confirm a generalized Harned law. The data were analyzed according to the primitive model of Friedman \(^{(2)}\) and interpreted in terms of the various interaction potentials \(^{(3)}\).

REFERENCES:
2. Friedman, H.L., J. Solution Chem. \( _1 \), 419 (1972) and refs. cited therein.

DETERMINATION OF ION-SOLVENT INTERACTION IN MIXED SOLVENTS FROM CONDUCTANCE MEASUREMENTS

D. Ilzycer and J. Padova

The conductances of cesium bromide and sodium bromide were determined at 25°C in mixtures of ethanol with water (10, 20, 40, 60 and 80% ethanol) from 0.001 molar up to near saturation. These measurements were carried out on a Shedlovsky bridge\(^{(1)}\) which has already been described\(^{(2)}\). Density and viscosity measurements needed for completion of the data were obtained at 25°C from a specially designed pycnometer and viscosimeter. The Bjerrum association constant \(^{(3)}\)

\[
K_A = \frac{4\pi N}{1000} \int_{a}^{q} r^2 \exp \left( -\frac{e^2 Z_+ Z_-}{ekT} \right) dr
\]

was interpreted in terms of Justice's equation\(^{(4)}\) and Fuoss's new theory\(^{(5)}\). The comparative study of these procedures\(^{(6)}\) leads to similar values for the dissociation constants \( K_A \). From these values, free energies of transfer of electrolytes from water to the mixed solvents or "medium effects" \(^{(7)}\) may be obtained as a further check on the accuracy of the data.

Experimental work is being continued.

REFERENCES:
1. Shedlowsky, T.J., Amer. Chem. Soc. \( _52 \), 1793 (1930)
Studies of the behavior of the dielectric constant (\(\varepsilon\)) of the nitrobenzene-n-hexane mixture at incipient phase separation were continued. Besides the peak in the dielectric constant that was reported earlier\(^{(1)}\), differences \(\Delta \varepsilon\) in the value of \(\varepsilon\) before and after separation were observed. This difference is positive when the nitrobenzene (NB) concentration is greater than the critical concentration \((\chi_{NB} = 0.428)\), and negative when it is less. The difference between the two values of \(\varepsilon\) is proportional to the difference between the actual concentration and the critical concentration:
\[
\Delta \varepsilon / \varepsilon = 1.5 (\chi - \chi_c) \quad \text{over the concentration range 0.38 - 0.46. Outside this range dependence on } (\chi - \chi_c) \text{ becomes weaker. This change in } \varepsilon \text{ can be explained in the following way. Consider a mixture of concentration } \chi \neq \chi_c \text{ at a temperature above separation temperature. On crossing the co-existence curve the mixture separates into two phases, one with concentration practically equal to } \chi_c \text{, and one with concentration } \chi', \text{ conjugate to } \chi. \text{ A simple calculation shows that } \Delta \varepsilon \text{ changes sign at } \chi = \chi_c, \text{ provided that the dependence of } \varepsilon \text{ on the composition has an inflection point around } \chi_c. \text{ Experiments are now in progress to investigate whether this inflection point exists.}
\]

The peak that appears at the critical concentration is finite; \(\varepsilon\) does not diverge. The non-divergence of \(\varepsilon\) may be explained as follows\(^{(2)}\). Fluctuations in the concentration of the more polar constituent, \(\delta c_1\) near the critical temperature \(T_c\) may cause a change in both the polarizability \(\alpha\) and the local field \(E_{\text{loc}}\). The change in the local dipole moment in the z-direction at the distance \(r\), \(\delta \mu_z = \delta (\alpha E_{\text{loc}}(r))\), can be taken as proportional to \(\delta c_1(r)\). The resulting dipole-dipole correlation function can be approximated as:
\[
<\delta \mu_z(0) \delta \mu_z(r)> \approx \alpha \delta c_1(0) e_z(0) \delta c_1(r) e_z(r)
\]
\[
\nu \quad <\delta c_1(0) \delta c_1(r)> <e_z(0) e_z(r)> \quad (1)
\]

where \(e_z(0)\) and \(e_z(r)\) are unit vectors related to the changes in direction of \(E_{\text{loc}}\) at \((0)\) and \((r)\). The concentration term in (1) becomes long-range.
at $T_c$, whereas no long-range correlation of the direction of $E_{\text{loc}}$ and its changes is to be expected. Therefore we may use, e.g., an Ornstein-Zernike expression for the concentration term and a decaying exponential for the directional term:

$$x_{zz} = (kT)^{-1} \int d^3r \langle \delta z(0) \delta z(r) \rangle$$

$$\propto (kT)^{-1} \int r^2dr \frac{e^{-kr}}{r} e^{-r/L} = [kT(\kappa+1/L)^2]^{-1}$$

and since $\kappa = |T-T_c|^\gamma$, the result is a finite peak. It may be pointed out that Mistura (3) has arrived at similar conclusions by different arguments.

REFERENCES:

STUDY OF LANTHANIDE CHLORIDE - ALIPHATIC ALCOHOL SYSTEMS
V. Tuler and M. Zangen

A series of experiments were carried out in order to ascertain whether so-called saturated solutions of anhydrous lanthanide chlorides in aliphatic alcohols are really solutions or, instead, liquid addition compounds.

As it was possible that the large discrepancies found in the literature data on solubility of lanthanide chlorides might be due to insufficient purity of the reagents, the solvents were checked by gas liquid chromatography, cryoscopy and Karl-Fisher analysis (the latter for dryness).

It was found, however, that the discrepancies might be due rather to insufficient equilibration. Even after several weeks of contact and mixing, the solution does not reach saturation, which is obtained only by vacuum evaporation of the free solvent after mixing at slightly elevated temperature. The high concentrations of lanthanide chlorides obtained in this latter manner would seem to support the "addition compound" theory.

AMINE EXTRACTION OF SILVER CHLORIDE COMPLEXES
M. Zangen

The partition of silver between aqueous chloride solutions of varying acidity and o-xylene solutions of trilaurylammonium chloride in various concentrations was determined radiometrically.
Treatment of the obtained partition data as a function of amine salt concentration and aqueous acidity by an appropriate computer program showed that:

a) the amine salt acts as a liquid anion exchanger for all the known silver chloride anions: $\text{AgCl}_2^-$, $\text{AgCl}_3^-$ and $\text{AgCl}_4^-$.

b) not only the monomer, but also the trimer and possibly the higher aggregate (n=50) of trilaurylammonium chloride participate in the extraction of silver species.

c) at least one water soluble complex is formed between the silver ion and trilaurylamine, i.e. $\text{Ag(C}_{12}\text{H}_{25}\text{NH}_{3})_2^+$, analogous to the known $\text{Ag(NH}_3)_2^+$.

CRYSTALLIZATION OF CALCIUM SULFITE

A. Cohen and M. Zangen

A series of experiments were carried out in order to obtain, in pure form, the various modifications of solid calcium sulfite previously postulated \(^{(1)}\).

Use was made of an H-shaped tube, one leg of which contained calcium chloride and the other sodium sulfite, while the connecting bridge contained either pure water or aqueous sodium chloride solutions of various concentrations. Diffusion of calcium and sulfite into the bridge caused their concentrations there to increase until the solubility product of calcium sulfite was reached, after which precipitation occurred.

The diffusion rate was found to be highly dependent on the concentration of sodium chloride in the bridge. When the latter contained originally only pure water, several months passed before any appreciable amount of precipitate was found. With a 3M solution of NaCl in the bridge, rapid diffusion of sodium ions into the calcium chloride leg occurred causing a compensatory movement of calcium ions through the bridge, so that the precipitation of calcium sulfite took place mostly in the sodium sulfite leg.

A preliminary X-ray investigation of crystals obtained in different media tends to support the previous conclusion \(^{(1)}\) concerning different modifications of calcium sulfite.

REFERENCE:

CALCULATION OF ISOHERMAL VAPOR-LIQUID EQUILIBRIUM DATA FOR BINARY MIXTURES FROM HEAT OF MIXING
M. Gazith

Heats of mixing (1), obtained by the use of a commercial titration calorimeter, were compared with values calculated using two parameter equations developed by Wilson (2,3) and Renon and Prausnitz (4-6). The heats of mixing along with vapor pressures, composition of liquid and vapor, and activity coefficients, were calculated from the data by computer. Graphs were prepared from the computer results of the calculated vs experimental data of heats of mixing. Also the calculated activity coefficients of a series of solvents and a non-volatile solute (tri-N-dodecyl amine) and vapor pressures of the solvents were plotted. Measurements of the latter can be done experimentally, in order to compare data thus obtained with the calculated results.

REFERENCES:

MOLAR VOLUMES OF ELECTROLYTES AND IONIC RADII BY LONG RANGE EXTRAPOLATION
M. Gazith

Intrinsic molar volumes of alkali halides were derived by long-range extrapolation (1-3) of densities of aqueous electrolyte solutions (4), based on concentration, and of molten salts, based on temperature (5). The adjusted intrinsic molar volumes of a hypothetical supercooled liquid salt at 25°C was found to be in good agreement with results obtained by compressibility (6-7) and other methods.

A randomly distributed hard sphere model with a packing coefficient of 4.35 (8) was ascribed to the pure electrolyte. A consistent set of ionic radii, in good agreement with standard values for the ion crystal radii (9) was obtained.
An examination was made of various models proposed for the correlation between ionic radii and molar volumes.

REFERENCES:

HYSTERESIS PHENOMENA AT THE CHARGE CYCLES OF THE DOUBLE LAYER OF ELECTRODES
M. Yaniv and A. Soffer

The potential-charge curves of the electrical double layer of electrodes are generally expected to be reversible. This assumption is mainly based on the excellent reversibility of the double layer of the dropping mercury electrode which persists even in cases of strong specific adsorption. This should not be the case if some surface chemical changes are involved in the charging process.

It has been proved earlier(1) that such surface chemical changes are equivalent to an appropriate double layer charging process. Since chemical processes may require an activation energy which, in the case of electrode processes, may be overcome by an overvoltage, hysteresis should appear in a charge-potential curve obtained by alternately raising and lowering the electrode potential.

The term surface chemical change stands for specific adsorption of dehydrated ions and surface oxide formation and decomposition. In cases of semi-conductor electrodes, this term is also valid for activated transfer of an electron from the conduction band of the solid electrode to a separate surface state and vice versa.

In the present work, hysteresis loops appearing in charge curves of a high surface carbon electrode were measured taking solutions of HCl, NaOH and especially NaCl at various pH values. Changes in pH of the solution during charge-discharge cycles were followed. The results were interpreted
in terms of the domain theory of hysteresis\(^{(2,3)}\). Various mechanisms which might cause hysteresis were considered. Charge transfer to electronic surface states conjugated to various surface groups seems to be responsible for hysteresis.

REFERENCES:

ELECTROCHEMICAL APPLICATION OF PARAMETRIC PUMPING
A. Soffer

The countercurrent column is a well established method for multistage continuous separation of a mixture. This process involves two fluid phases streaming in countercurrent. Many solids are selective adsorbents and could serve as efficient separators but, since they cannot be readily fluidized, they are unsuitable for multistage countercurrent separation.

A new cyclic method, not yet utilized industrially, has recently been suggested\(^{(1)}\), by which cycles of adsorption-desorption on a solid adsorbent are conjugated with cyclic movement of the fluid along the column. By this regime, which is called parametric pumping, a multistage separation process can be transformed into an adsorption column containing only one movable fluid phase. The second phase is a solid fixed within the column.

A serious disadvantage of this method is the large amount of thermal energy needed to induce desorption. This limitation could be overcome by using a more specific intensive parameter whose energy demand for transferring material between solid and fluid is, unlike heat, not much higher than the thermodynamic free energy of the process.

The electrical potential in reversible electrode processes is such a specific parameter which can induce efficient transfer of electroactive materials from the solution to the electrode. A porous electrode of high surface area can serve as a high capacity solid phase, while the pronounced selectivity of the electrode process provides the separation power.
An electrochemical column operated for multistage separation is suggested. This column is to be filled, side by side with a porous electrode, an electrode separator and a counter electrode.

Electrode processes are utilized industrially only in batch or single stage techniques and there are only a few research studies on column electrodes.

The assembly suggested, which may be called an "electrochemical parampump", combines the parametric pumping principle together with electrochemical processes and permits the utilization of electrochemistry for continuous multistage separation methods.

A theoretical study of the performance of the electrochemical parampump in the separation of a mixture of ionic isotopes was carried out. Expressions were derived for the height of the theoretical plate and the net transport of isotope during one cycle of operation. The conditions for optimal operation of the column were considered in terms of the separation work. The results obtained closely resemble the expressions of normal countercurrent columns operating with two fluids streaming unidirectionally.

REFERENCES:

ELECTROLYTIC SYNTHESIS OF SINGLE AND MIXED ORTHORHOMBIC OXIDES
M. Zafrir, L. Bendor*, R. Zilber and A. Aladjem

Further research was carried out on the electrolytic synthesis of single and mixed orthorhombic oxides. The cases of $\text{U}_3\text{O}_8$, $\text{Ta}_2\text{O}_5$ and $\text{Nb}_2\text{O}_5$ are treated here as illustrative examples.

Uranium, tantalum or niobium (in the form of high-purity foil 0.1-0.2 mm thick) was made the anode in a single-cell electrolyzer; platinum wire was used as the cathode. Tantalum or niobium can also be used as the cathode but attempts to use an uranium cathode failed because of rapid hydrogenation. In the preparation of mixed oxides, the two metals can be used simultaneously as the anode, but better composition control is achieved by consecutive dissolution of the metals.

* Hebrew University, Jerusalem
The electrolytes used were solutions of ammonium chloride or ammonium nitrate in methanol. The electrolysis was carried out under the following conditions: room temperature, continuous agitation by magnetic stirrer, 20 V applied voltage, 100 mA/cm² anodic c.d.

In the dissolution of tantalum and niobium the anodic current efficiency was >100%; in the dissolution of uranium the efficiency was not measured with accuracy because of partial losses of metal due to mechanical disintegration.

The thermal decomposition of the electrolyte has been described previously. The product oxides (single or mixed) were in the form of a fine powder, and in each case the structure was orthorhombic (as determined by X-ray diffraction). The cell parameters are given in Table 2 (in angstrom units).

<table>
<thead>
<tr>
<th>Oxide Parameter</th>
<th>U₃O₈</th>
<th>Ta₂O₅ (from chlorine)</th>
<th>Nb₂O₅ (from nitrate)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>4.142</td>
<td>6.212</td>
<td>6.170</td>
</tr>
<tr>
<td>b</td>
<td>6.744</td>
<td>3.643</td>
<td>3.661</td>
</tr>
<tr>
<td>c</td>
<td>3.964</td>
<td>3.879</td>
<td>3.935</td>
</tr>
</tbody>
</table>

The crystallographic data show that the electrolyte (chloride or nitrate) had virtually no effect on the structure of the final product; mixed Ta₂O₅-Nb₂O₅ oxides were orthorhombic and their lattice parameters varied regularly with variations in the Ta:Nb ratio (e.g., the parameter c increased linearly in the transition from Ta₂O₅ to Nb₂O₅, while the changes in the other parameters were regular but not linear.

REFERENCE:

OVERFARADIC EFFECT IN THE ELECTROLYTIC DISSOLUTION OF COLD-ROLLED ZIRCALOY-2
A. Aladjem and G. Gafni

Electrolytic dissolution of Zircaloy-2 is potentially of importance for nuclear technology, in view of the extensive use of Zircaloy-2 and other...
high-zirconium alloys (Zircaloy-4, Zr-Nb) as a cladding and structural metal in power plant reactor cores. Electrolytic dissolution involves non-corrosive solvents, is easily controlled, and minimizes undesirable attack on structural metals. It may be used for cladding surface treatment (to remove surface flaws such as microcracks), cladding dissolution for subsequent chemical or spectroscopic analysis, deburring, weld surface smoothening, etc.

We have developed an improved electrolytic dissolution technique for Zircaloy-2. Zircaloy-2 sheet, 1.1 mm thick, was cold rolled in 30 passes to a thickness of 0.15 mm, and the resulting foil was used as the anode in a cell containing a saturated solution of ammonium chloride in methanol to which 4 cm$^3$ of conc. HCl per liter was added. The addition of HCl improved the uniformity of dissolution. Carbon steel was used as the cathode, and the dissolution was carried out at ambient temperature with simultaneous voltage and current control.

One of the most important parameters for controlling the electrochemical dissolution of metals is the faradaic current (anodic) efficiency, i.e. the ratio of the experimentally determined weight loss for a given current-time product to the theoretical (faradaic) loss: $\eta\% = (\frac{Ag_{\text{exp}}}{Ag_{\text{far}}}) \times 100$.

In the dissolution of Zircaloy-2 we consistently observed an overfaradaic effect, i.e., the current efficiency was substantially higher than 100%. Typical results obtained with samples of a single batch of cold-rolled Zircaloy-2 at different anodic current densities are listed in Table 3.

<table>
<thead>
<tr>
<th>Total current mA-min</th>
<th>Current density mA/cm$^2$</th>
<th>Weight loss, mg</th>
<th>Overfaradaic effect, % above theor. current efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>80</td>
<td>16.13</td>
<td>14.10</td>
</tr>
<tr>
<td>3000</td>
<td>80</td>
<td>50.20</td>
<td>42.30</td>
</tr>
<tr>
<td>3000</td>
<td>80</td>
<td>54.19</td>
<td>42.30</td>
</tr>
<tr>
<td>1500</td>
<td>40</td>
<td>24.14</td>
<td>21.15</td>
</tr>
<tr>
<td>1500</td>
<td>40</td>
<td>23.43</td>
<td>21.15</td>
</tr>
<tr>
<td>3000</td>
<td>240</td>
<td>46.56</td>
<td>42.30</td>
</tr>
</tbody>
</table>

TABLE 3
Calculated and experimental weight losses in the electrolytic dissolution of Zircaloy
In previous experiments, we found that the dissolution of pure, annealed metals also involves an overfaradaic effect, but of much lower magnitude, e.g., 3-4% or less in the case of pure zirconium. The effect in Zircaloy is almost an order-of-magnitude greater, and seems to be c.d.-dependent, with a peak at ~80 mA/cm².

Thus, a new technique for the electrochemical dissolution of Zircaloy-2 has been developed. The linear dissolution rates achieved by this technique were 60-480 μm/h. The dissolution proceeds with very high (relative to pure annealed metals) overfaradaic effects. The nature of the overfaradaic effect is now being investigated; it is assumed that it is associated with internal stresses and inhomogeneity of the alloy, and probably involves mechanical and chemical losses of metal.

TREATMENT OF CYANIDE WASTES
R. Rafaeloff, J. Padova and L. Cohen

A method was developed for the recovery of copper, zinc, cadmium and silver from cyanide wastes and the electrolytic oxidation of cyanides. The method includes the following steps:

a. loading an ion exchange column with cyanide wastes containing cyanide complexes of the above metals and free cyanide
b. elution of the loaded compounds from the ion exchange column
c. electrolytic destruction of the cyanide from the element and simultaneous cathodic deposition of the metals mentioned.

The process is reasonably efficient, which is encouraging for further investigation under large scale conditions.

REFERENCES:

SOLVENT MEMBRANE SEPARATION
Z. Ketzinel, Z. Boger and H. Cikurel

In continuation of previous work additional experiments were performed to investigate the possible use of solvent-type membranes in the first cycle separation of enriched uranium from U-Al alloy fuel elements. The research was carried out together with Prof. D. Vofsi, head of the plastics laboratory of the Weizmann Institute, where the solvent membranes were developed.
The feed solution in the present tests was a simulated uranyl nitrate - aluminium nitrate solution containing fission product tracers at mCi/l levels. Inactive fission product elements were added in amounts equal to the calculated concentrations in a real fuel element solution that would result from the IRR-1 pool type research reactor at Soreq. Experiments showed a decontamination factor for gamma emitters on the order of several hundreds.

The product solution from the membrane module was further purified by a second membrane module, after dissolution of aluminium nitrate crystals to get the desired salting-out strength. In this second cycle a decontamination factor of several tens was achieved, thus resulting in an overall process decontamination factor of several thousands for gamma emitters.

The residual uranium in the waste solution was recovered and purified by passage through another membrane module, thus reducing the total uranium loss to 0.2%, relative to the feed solution.

Pending a hot-cell test with full activity simulated solutions to verify the actual decontamination factor and the expected life-time of the module under radiation, a simple scheme (see Fig. 5) was designed to process one irradiated fuel element per day, giving a semi-purified uranyl nitrate solution that could be further processed without heavy shielding.

**Fig. 5**

Diagram of the separation process

1) feed: Al, U, F.P. nitrates
2) H₂O
3) waste Al, F.P. nitrates
4) 1st cycle product: U nitrate
5) solid Al(NO₃)₃·9H₂O
6) 2nd cycle feed: Al, U nitrates
7) waste: Al, F.P. nitrates, trace U
8) 2nd cycle product

**REFERENCE:**

SOLVENT MEMBRANES BASED ON AMIDE PLASTICIZED POLYMERS
M.S. Dariel

Halcomides are industrial polysubstituted amides with a very high (>50% w/v) capacity for absorbing water. A marked temperature dependence of the absorption of water, combined with the low solubility of chlorides in the amides, suggest they may be useful in desalination.

Difficulties in phase separation and entrainment of solvent can be avoided by adapting the amide to a membrane separation process. Solvent membranes (40 microns thick), prepared by plasticizing suitable polymers, were found to be almost impenetrable to sodium chloride. Water flux in an osmotic gradient of 0.3M NaCl was 0.5x10^{-6} cm sec^{-1} and in a thermal gradient of 30°C was 0.2x10^{-6} cm sec^{-1}.

Mechanical properties of the membranes were satisfactory. Further work is being directed toward the improvement of lifetimes and stability of the membranes.

PREPARATION OF GALLIUM (III) HALIDE COMPLEXES
A. Silberstein, Y. Weiss and R. Rafaeloff

In the present work a new series of gallium (III) halide complexes were prepared by mixing methanolic solutions containing stoichiometric amounts of the organic molecule and the gallium halogenides. On cooling, white crystalline compounds were obtained. The crystals were filtered and washed with absolute methanol and dried over P_{2}O_{5}. These compounds can be recrystallized from absolute methanol.

The following compounds were prepared:

\[
\begin{align*}
[(\text{CH}_3)_3\text{C}_6\text{H}_5\text{N}]^+ [\text{GaBr}_3\text{Cl}]^- & \quad \text{m.p. 149°C} \\
[(\text{CH}_3)_3\text{C}_6\text{H}_5\text{N}]^+ [\text{GaCl}_4]^- & \quad \text{m.p. 203°C} \\
[(\text{C}_6\text{H}_5)_4\text{P}]^+ [\text{GaCl}_4]^- & \quad \text{m.p. 208°C} \\
[(\text{C}_6\text{H}_5)_4\text{P}]^+ [\text{GaBr}_3\text{Cl}]^- & \quad \text{m.p. 76°C} \\
[(\text{C}_6\text{H}_5)_4\text{P}]^+ [\text{GaBr}_4]^- & \quad \text{m.p. 71°C} \\
[(\text{C}_6\text{H}_5)_4\text{P}]^+ [\text{GaBr}_3\text{Cl}]^- & \quad \text{m.p. 201°C} \\
[(\text{C}_6\text{H}_9)_4\text{P}]^+ [\text{GaBr}_4]^- & \quad \text{m.p. 207°C} \\
[(\text{C}_6\text{H}_9)_4\text{P}]^+ [\text{GaBr}_3\text{Cl}]^- & \quad \text{m.p. 135°C} \\
[(\text{C}_6\text{H}_5)_4\text{As}]^+ [\text{GaCl}_4]^- & \quad \text{m.p. 183°C} \\
[(\text{C}_6\text{H}_5)_4\text{As}]^+ [\text{GaBr}_3\text{Cl}] & \quad \text{m.p. 189°C} \\
[(\text{C}_6\text{H}_5)_4\text{Sb}]^+ [\text{GaBr}_6]^- & \quad \text{m.p. 207°C} \\
[(\text{C}_6\text{H}_5)_4\text{Sb}]^+ [\text{GaBr}_3\text{Cl}]^- & \quad \text{m.p. 203°C}
\end{align*}
\]
RAMAN SPECTRA OF GALLIUM (III) HALIDE COMPLEXES
A. Silberstein and R. Rafaeloff

The Raman spectra of tetrachloro-, tetrabromo-, trichlorobromo- and tribromochloro-gallate anions were studied. The results support the $T_d$ symmetry for GaX$_4^-$ complexes$^{(1,2)}$, and $C_{3v}$ symmetry for the mixed halide complexes, GaBrCl$_3^-$ and GaBr$_3$Cl$^-$. There are two possible structures for the GaX$_3^-$Y$^-$ complexes. If the structure is GaX$_3^-$Y$^-$ (structure I) the symmetry is $C_{3v}$, for which group theory predicts 6 Raman active lines, 3 of them $e$ species and the other 3, $a$ species. If GaX$_3^-$Y$^-$ exists as a dimeric unit (structure II), the symmetry is $D_{2h}$ and 13 Raman frequencies are expected.

$$\begin{align*}
\text{I} & \quad \begin{bmatrix}
X \\
\downarrow \\
Y - Ga - X \\
\uparrow \\
X
\end{bmatrix}^- \\
\text{II} & \quad \begin{bmatrix}
X \\
\downarrow \\
X - Ga - Y \\
\uparrow \\
X
\end{bmatrix}^{-2}
\end{align*}$$

The number of lines and the relative intensities of the observed frequencies in the spectra indicate that the mixed halide compounds have the GaX$_3^-$Y$^-$ (I) structure. The data and assignments are summarized in Tables 4 and 5.

### Table 4

<table>
<thead>
<tr>
<th>Raman frequencies of GaX$_4^-$ (cm$^{-1}$)</th>
<th>(CH$_3$)$_3$C$_6$H$_5$N$^+$CaCl$_4^-$</th>
<th>(C$_4$H$_9$)$_4^+$GaBr$_4^-$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v_2$ (e)</td>
<td>117 (s)</td>
<td>70 (m)</td>
</tr>
<tr>
<td>$v_4$ ($f_2$)</td>
<td>152 (s)</td>
<td>100 (s)</td>
</tr>
<tr>
<td>$v_1$ ($a_1$)</td>
<td>346 (vs)</td>
<td>209 (vs)</td>
</tr>
<tr>
<td>$v_3$ ($f_2$)</td>
<td>380 (vw)</td>
<td>277 (w)</td>
</tr>
</tbody>
</table>
TABLE 5
Raman frequencies of GaX₃⁻ (cm⁻¹)

<table>
<thead>
<tr>
<th></th>
<th>((\text{n-C}_3\text{H}_7)_4\text{N}^+\text{GaCl}_3\text{Br}^-)</th>
<th>((\text{CuH}_9)_4\text{P}^+\text{GaCl}_3\text{Br}^-)</th>
<th>((\text{C}_4\text{H}_3)_3\text{P}^+\text{GaCl}_3\text{Br}^-)</th>
<th>((\text{C}_6\text{H}_5)_4\text{As}^+\text{GaBr}_3\text{Cl}^-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(v_6(e))</td>
<td>142 (m)</td>
<td>143 (m)</td>
<td>140 (w)</td>
<td>117 (sh)</td>
</tr>
<tr>
<td>(v_3(a_1))</td>
<td>246 (m)</td>
<td>245 (m)</td>
<td>243 (m)</td>
<td>212 (vs)</td>
</tr>
<tr>
<td>(v_2(a_1))</td>
<td>263 (m)</td>
<td>260 (s)</td>
<td>262 (m)</td>
<td>246 (vs)</td>
</tr>
<tr>
<td>(v_1(a_1))</td>
<td>348 (vs), 356 (sh)</td>
<td>348 (vs), 355 (sh)</td>
<td>346 (s), 354 (sh)</td>
<td>230, 234 (vs)</td>
</tr>
<tr>
<td>(v_4(e))</td>
<td>375, 380 (vw)</td>
<td>380 (m) 384 (sh)</td>
<td>377 (vw)</td>
<td>275 (m), 282 (sh)</td>
</tr>
</tbody>
</table>

(w)-weak, (m)-medium, (s)-strong, (sh)-shoulder, (v)-very

REFERENCES:

THE REACTION OF AMMONIUM PERTECHNETATE WITH ANHYDROUS HYDROGEN FLUORIDE:
VIBRATIONAL SPECTRA OF PERTECHNETYL FLUORIDE
J. Binenboym, U. El-Gad and H. Selig

Ammonium pertechnetate dissolves slightly in anhydrous hydrogen fluoride to give solutions of pertechnetyl fluoride. Raman spectra of the solutions as well as infrared and Raman spectra of the pure compound indicate that TcO₅F⁻ has a C₃ᵥ symmetry with the following assignments: \(a_1\): 696, 962 and 317 cm⁻¹; \(e\): 951, 347 and 231 cm⁻¹. A comparison with other MO₅X compounds indicates a necessity to reverse some of the original assignments.

REFERENCE:

SOME PHYSICAL PROPERTIES OF TECHNETIUM-99 PENTAFLUORIDE
J. Binenboym and H. Selig

Technetium pentfluoride was prepared from the hexafluoride by the reduction with iodine in iodine pentfluoride according to

\[ \text{IF}_5 + \text{I}_2 + 10 \text{TcF}_6 \rightarrow 10 \text{TcF}_5 + 2 \text{IF}_5 \]

* Hebrew University, Jerusalem
Raman spectra of liquid TcF\textsubscript{5} were measured and compared with those of MoF\textsubscript{5}, NbF\textsubscript{5} and TaF\textsubscript{5}. Attempts to obtain Raman spectra of solid TcF\textsubscript{5} were not wholly successful, because the solid absorbed enough energy from the laser beam to cause local melting. For solid TcF\textsubscript{5} at -50°C the bond stretching region is dominated by three strong sharp bands at 698, 750 and 775 cm\textsuperscript{-1} in addition to several weak ones. In this respect it resembles MoF\textsubscript{5} as well as NbF\textsubscript{5} and TaF\textsubscript{5}. Crystallographically TcF\textsubscript{5} belongs to a group of which VF\textsubscript{5} is the prototype, in which the units are linked in endless chains by cis-bridging via fluorine atoms. The similarity of the Raman spectra as well as other physical properties indicate that TcF\textsubscript{5} is polymerized in the liquid as well.

TcF\textsubscript{5} is only very sparingly soluble in anhydrous hydrogen fluoride and attempts to obtain Raman spectra of such solutions were unsuccessful. It is thus similar to MoF\textsubscript{5} which has been shown to be a very much weaker fluoride ion acceptor (Lewis acid) than SbF\textsubscript{5} and AsF\textsubscript{5}.

The magnetic susceptibility of TcF\textsubscript{5} was measured and a magnetic moment of 300 B.M. was found. The magnetic moment is thus close to the spin-only value for two non-bonding electrons and rather higher than that of analogous ReF\textsubscript{5} (μ ≈ 25 B.M.)

REFERENCE:

LUMINESCENCE OF MERCURY-LIKE ION CENTERS
B. Barnett, R. Reisfeld* and L. Boehm*

Absorption (\textsuperscript{1}S \rightarrow \textsuperscript{3}P\textsubscript{1}) and fluorescence (\textsuperscript{3}P\textsubscript{1} \rightarrow \textsuperscript{1}S\textsubscript{0}) spectra of Sn\textsuperscript{2+}, Sb\textsuperscript{3+} and Bi\textsuperscript{3+} in borax phosphate and germanate glass were measured at various temperatures. The fluorescence decay for Bi\textsuperscript{3+} in germanate glass was measured at 83° and 293°K and was found to be non-exponential at 293°K. Quantum efficiencies were obtained for the above ions and matrices.

These experimental results were interpreted using the configurational coordinate diagram model. The electronic levels included in the model were the ground \textsuperscript{1}S\textsubscript{0} and excited \textsuperscript{3}P\textsubscript{1} and \textsuperscript{3}P\textsubscript{0} levels. The effect of a Jahn-Teller splitting of the \textsuperscript{3}P\textsubscript{1} state was examined.

The non-exponential fluorescence decay was resolved into two exponential components related to the \textsuperscript{3}P\textsubscript{1} \rightarrow \textsuperscript{3}P\textsubscript{0} thermalization and \textsuperscript{3}P\textsubscript{1} \rightarrow \textsuperscript{1}S\textsubscript{0} radiation.

* Hebrew University, Jerusalem
MEASUREMENT OF FLUORESCENCE OF Nd$^{+3}$ IN MOLTEN SALTS

J. Hausman

The purpose of this work is to study the characteristics of fluorescence of Nd$^{+3}$ in molten nitrates. Special cells containing small amounts of Nd(NO$_3$)$_3$ in a NaNO$_3$-KNO$_3$ eutectic solution were prepared.

The cells are pumped by means of a N$_2$ laser and several dye lasers, which makes it possible to check the effectiveness of different absorption bands of the Nd$^{+3}$ in producing fluorescence. An S-1 type photomultiplier is used as a detector of the 1.06 fluorescence. The experimental set-up was checked by measuring the fluorescence in Nd glass. The measurements of fluorescence of Nd$^{+3}$ in molten salts are in progress.

EXPERIMENTAL INTERACTION DIPOLES FOR THE RARE GASES

E. Bar-Ziv and S. Weiss

Interaction dipoles for He-Ar, He-Kr, He-Xe, Ne-Ar, Ne-Kr, Ne-Xe, Ar-Kr, and Ar-Xe were determined (Fig. 6) by adjusting the parameters of flexible
### TABLE 6
Interaction dipole parameters for the various rare gas pairs

<table>
<thead>
<tr>
<th>Pair</th>
<th>$\alpha_1$ (debye)</th>
<th>$\alpha_2$ (debye)</th>
<th>$\alpha_3$ (debye)</th>
<th>$\alpha_4$ (debye)</th>
<th>$\alpha_5$ (debye)</th>
<th>$\mu$ (debye)</th>
<th>$\frac{C_1}{\lambda}$</th>
<th>$\frac{C_2}{\lambda}$</th>
<th>$\lambda$</th>
<th>$\rho / \alpha_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>He–Ar</td>
<td>123.58</td>
<td>2578.6</td>
<td>139.97</td>
<td>16.165</td>
<td>15.824</td>
<td>-0.74813</td>
<td>373.0</td>
<td>-5.535</td>
<td>3.00</td>
<td>2.61</td>
</tr>
<tr>
<td>He–Kr</td>
<td>-294.44</td>
<td>3637.0</td>
<td>186.79</td>
<td>-15.763</td>
<td>-17.981</td>
<td>0.36994</td>
<td>523.8</td>
<td>-5.640</td>
<td>3.09</td>
<td>2.69</td>
</tr>
<tr>
<td>He–Xe</td>
<td>827.11</td>
<td>2572.8</td>
<td>2677.7</td>
<td>211.12</td>
<td>104.06</td>
<td>-6.5388</td>
<td>746.9</td>
<td>-14.522</td>
<td>3.36</td>
<td>2.29</td>
</tr>
<tr>
<td>Ne–Ar (B)</td>
<td>-281.34</td>
<td>3880.0</td>
<td>178.06</td>
<td>-24.925</td>
<td>-22.475</td>
<td>1.38295</td>
<td>479.1</td>
<td>-5.554</td>
<td>3.10</td>
<td>2.70</td>
</tr>
<tr>
<td>Ne–Kr</td>
<td>-338.33</td>
<td>4458.9</td>
<td>206.42</td>
<td>-25.600</td>
<td>-25.869</td>
<td>1.8399</td>
<td>396.8</td>
<td>-4.227</td>
<td>3.10</td>
<td>2.70</td>
</tr>
<tr>
<td>Ne–Xe</td>
<td>-1375.90</td>
<td>21406</td>
<td>-278.55</td>
<td>-69.833</td>
<td>-38.036</td>
<td>4.3048</td>
<td>544.2</td>
<td>-7.450</td>
<td>3.19</td>
<td>2.78</td>
</tr>
<tr>
<td>Ar–Kr</td>
<td>-4149.50</td>
<td>51710</td>
<td>-513.67</td>
<td>-101.22</td>
<td>-55.267</td>
<td>4.2510</td>
<td>801.7</td>
<td>-20.03</td>
<td>3.46</td>
<td>3.01</td>
</tr>
<tr>
<td>Ar–Xe</td>
<td>-2321.80</td>
<td>26228</td>
<td>-247.91</td>
<td>-74.363</td>
<td>-34.998</td>
<td>3.6077</td>
<td>314.3</td>
<td>-2.922</td>
<td>3.52</td>
<td>3.06</td>
</tr>
</tbody>
</table>

*aDipole based on the results of Bosomworth and Gush [Ref. 2] according to our present procedure.

*bDipole based on the results of Bosomworth and Gush, according to our former procedure (Ref. 3). Dipole based on the results of Quazza and Marteati (Ref. 4) according to our present method.
dipole moment functions to reproduce the experimental collision-induced translational spectra (Fig. 7). The parameters $a_4$ are collected in Table 6.

Fig. 7

Experimental spectra (solid) and calculated spectra (dashed). Parts of spectra extrapolated according to Levine and Birnbaum(5), are dotted (He-Kr and He-Xe). For Ne-Ar two spectra are shown: results of Bosomworth and Gush(2) (I) and those of Quazza and Marteau(4) (II). Two calculated spectra, both corresponding to the results of Bosomworth and Gush (one according to our former procedure(3) and one according to our present procedure), are indistinguishable.

REFERENCES:
4. Marteau, P. and Quazza, J. (J. Quazza, thesis (University of Paris, 1972)) (Measured Ne-Ar, Ne-Kr, Ne-Xe, Ar-Kr, and Ar-Xe)
REARRANGEMENT OF EPOXIDES BY HOMOGENEOUS CATALYSIS OF THE GROUP VIII METAL COMPLEXES
D. Milstein, J. Blum * and O. Buchman

Extensive literature has been published in the field of homogeneous catalysis by transition metal complexes. Few of the publications refer to the possibility of C-O bonds opening by such complexes.

We found that in different epoxide derivatives the catalyst breaks the epoxide C-O bond. The resulting products are characterized by a structural rearrangement involving a carbonyl group. Some representative complex reactions with trans-stilbene oxide are given in Table 7.

TABLE 7
Catalytic effect of metal complexes on trans-stilbene oxide

<table>
<thead>
<tr>
<th>cis-stilbene oxide</th>
<th>trans-stilbene oxide</th>
<th>trans-stilbene</th>
<th>diphenylmethane</th>
<th>diphenylacetaldehyde</th>
<th>deoxybenzoin</th>
<th>catalyst</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>%</td>
<td>%</td>
<td>%</td>
<td>%</td>
<td>%</td>
<td></td>
</tr>
<tr>
<td>0.3</td>
<td>0</td>
<td>2.8</td>
<td>7.9</td>
<td>0</td>
<td>87.9</td>
<td>ClRh(PPh₃)₃</td>
</tr>
<tr>
<td>0.8</td>
<td>0</td>
<td>3.5</td>
<td>3.4</td>
<td>0</td>
<td>80.2</td>
<td>ClRh(CO)(PPh₃)₂</td>
</tr>
<tr>
<td>0.1</td>
<td>0</td>
<td>3.8</td>
<td>1.8</td>
<td>10.1</td>
<td>40.8</td>
<td>RuCl₂(PPh₃)₃</td>
</tr>
<tr>
<td>0.3</td>
<td>18.3</td>
<td>12.1</td>
<td>11.3</td>
<td>25.1</td>
<td>8.2</td>
<td>[Rh(CO)₂Cl]₂</td>
</tr>
<tr>
<td>0.2</td>
<td>0</td>
<td>16.3</td>
<td>8.8</td>
<td>0</td>
<td>34.7</td>
<td>ClIr(CO)(PPh₃)₂</td>
</tr>
</tbody>
</table>

To interpret these results, two different mechanisms may be proposed. The first includes the intermediate step (I) in which the metal subsists with a d⁸ configuration. Such a mechanism is similar to Lewis acid catalysis and leads to the aldehyde. The second mechanism involves oxidative addition and the intermediate step (II) in which the hydride migration leads to the ketone.

\[
\begin{align*}
\text{(I)} & \quad \text{H} \quad \text{R} \quad \text{C} \quad \text{C} \quad \text{H} \\
\text{O} \quad \text{-(Rh)I}^- \\
\text{(II)} & \quad \text{H} \quad \text{R} \quad \text{C} \quad \text{C} \quad \text{H} \\
\text{(Rh III)O} 
\end{align*}
\]

REFERENCES:

* Hebrew University, Jerusalem
CATALYTIC HYDROGENATION OF ALDOXIMES
D. Milstein, M. Blitzblau and O. Buchman

In continuation of previous research\(^{(1)}\), the solvent effect on furfur-aldoxime hydrogenation, below atmospheric pressure, was investigated. A lower reaction rate was found in dioxan than in methanol (Fig. 8). A higher maximum in the furfurylamine formation was reached with the syn isomer.

**Fig. 8**
Solvent effect on furfuraldoxime hydrogenation with Raney nickel at 400 Torr

In the case of benzaldoxime hydrogenation in methanol (Fig. 9) similar behavior of the syn and anti isomers was observed.
Fig. 9
Hydrogenation of furfur- and benz-aldoximes with Raney nickel at 600 Torr

REFERENCE:
C. Shenberg and S. Amiel

Different methods of correction for interelement effects in X-ray fluorescence analysis, as applied to two-element samples, were examined and evaluated. These correction methods were applied to the determination of Cu in Cu-Fe solutions and solids. The methods of calculation based on the $\alpha$ correction factor were checked over a wide range of Cu and Fe concentrations with the result that the $\alpha$ factor was found to vary considerably. Introducing peak ratios instead of intensity into the $\alpha$ correction method formula was found to extend this method over a wider range of concentrations, but it is limited to samples of the same chemical composition as the standards.

The original peak ratio method of correction was found to be independent of both the concentration range and chemical composition; accuracies of 3.5% were obtained with samples containing two main elements. This was compared with 4.0% error obtained when the $\alpha$ modified correction method was used for samples of the same chemical composition as standards. The error was about 50% for samples of different chemical composition than standards. The original $\alpha$ method gave even greater errors and therefore cannot be applied to the concentration range covered by the peak ratio method.

REFERENCES:

C. Shenberg, A. Ben Haim and S. Amiel

In a solution containing a single predominant element, the ratio of an X-ray fluorescence line to a target backscattered line varies linearly with the concentration of the element over a wide range. However, the presence of an additional component of lower $Z$ distorts the proportionality. We have shown that accurate analysis can be carried out in mixtures by suitable treatment of the data.

A rough estimate of the lower $Z$ component was obtained by the usual peak ratio method. The ratio of its fluorescence line to the target back-
scattered line was largely independent of the concentration of the higher Z component. This fact and a comparison of mixture solutions of various concentrations with single-element solutions of similar concentrations permitted correction for the distortion introduced by the presence of the lower Z element. The case studied was the mutual influence of Cu and Fe on the ratios between the fluorescent K X-rays of the individual elements and the backscattered target X-rays in various Cu-Fe mixtures. The X-rays were excited using a 241Am-As source-target assembly and measured with a Si(Li) detector. Using the new method of calculation, satisfactory analytical results were obtained for solutions of 0.6 to 25 w/v % Cu in the presence of 0.4 to 23 w/v % Fe. The procedure was extended to solid mixtures and ores containing up to 80% Cu.

REFERENCE:

DETERMINATION OF YTTRIUM IN PHOSPHATE ROCKS BY NEUTRON ACTIVATION FOLLOWED BY X-RAY SPECTROMETRY
M. Mantel and S. Amiel

Reactor neutron activation followed by high resolution X-ray spectrometry was applied to the nondestructive determination of yttrium in phosphate rocks.

The Y X-rays emitted following internal conversion during the decay of 90mY (obtained from 89Y by neutron activation) were measured with a 100 mm² Si(Li) spectrometer. A sensitivity of 1 dps/µg was found for a 5 min irradiation, a thermal neutron flux of 10¹³ n/cm² sec and an overall geometry of 4% (1). Due to this relatively high sensitivity, it was possible to use short irradiation times and measure the emitted X-rays through a 2.0 mm plastic absorber. In this way the interference of the strong bremsstrahlung, due to the presence of a large quantity of P in the sample, was overcome.

Concentrations of 20-50 ppm Y in phosphate rocks were determined with an overall error of ±2%.

REFERENCE:

DETERMINATION OF GALLIUM IN CLAYS BY NEUTRON ACTIVATION ANALYSIS
A. Padova and O. Even

Traces of gallium in clays were determined by neutron activation analysis using a high resolution lithium-drifted germanium detector. The principal
835 keV gamma ray of $^{72}$Ga was measured with a 60 cm$^3$ Ge(Li) spectrometer in conjunction with a Packard 4000 channel analyzer and Wang table computer, model 720 C. Samples were weighed into polyethylene bags, sealed and inserted into polyethylene vials. Gallium metal and gallium oxide used as standards were similarly prepared for irradiation. The sample and the standards were irradiated simultaneously (in one rabbit) for 10 minutes at a flux of $3.5 \times 10^{12}$/n cm$^2$ sec. Careful calibration of the spectrometer and judicious choice of cooling time eliminate the influence of such elements as $^{152m}$Eu (841 keV) and $^{24}$Na, and make possible the determination of gallium without prior chemical separation. Under these conditions, the detection limit was found to be 0.1 µg for a 100 mg clay sample.

USE OF ACTIVATION ANALYSIS FOR DETERMINATION OF CALCIUM IN THE PRESENCE OF SODIUM IN AIR FILTERS
A. Padova and O. Even

Neutron activation analysis was applied to determine traces of calcium in the presence of at least twenty times as much sodium in air filters. The procedure involves ignition of the filter in a quartz ampoule, then irradiation for 10 hours with thermal neutrons at a flux of $10^{13}$/n/cm$^2$ sec. Two days later the ampoule is opened and the ash dissolved in HCl. Calcium is then separated from sodium by one of the following methods:

a) precipitation of calcium as oxalate
b) separation of sodium on an HAP ion exchange column

The separated calcium is then determined by counting with a Ge(Li) counter. Using this method, as little as 50-100 µg calcium can be determined.

DETECTION OF GUNSHOT RESIDUES*
A. Padova, O. Even and E. Yellin

Gun powder and primers from Israeli made ammunition were analyzed by neutron activation. The powder was found to contain Al, Sn, K and Fe in significant concentrations. The primers were found to contain Sb, K and Cl. No Ba was observed in the primers.

A technique was developed for collecting traces of gunshot residues by applying a cellulose acetate film on human body surfaces. The film is easily applied and readily removed. Then neutron activation analysis is used to resolve the trace elements.

*The investigation is supported by the Israel Police
Work is continuing towards the development of a method for the identification of a suspected gunman based on residue analyses.

DETERMINATION OF LITHIUM IN BRINES AND POLAR SOLVENTS BY ATOMIC ABSORPTION SPECTROPHOTOMETRY

R. Levin

Problems connected with the extraction of lithium from brine prompted Ben-Zwi\(^1\) to look for improvements in the analysis of lithium in organic solvents used in the extraction process. The standard addition method, applied to solvents, is often inconvenient due to the volatility of the solvent and the necessity of using a large number of vessels. In addition, when more than one solvent is tested in the process of extraction of lithium from brines, standard absorption curves have to be prepared for each solvent separately.

We investigated lithium solutions in butanol, isopropanol and propylene carbonate. In all cases a 1:1:1 homogeneous solution could be obtained with ethanol and water. The mixture thus obtained could be treated as a quasi-aqueous solution. It was very simple to apply the standard procedure to these solutions using purely aqueous standard additions.

On the other hand, in cases where the lithium content was high it was possible to dilute the 1:1:1 mixture with water and when this dilution could be made extensive it was possible to compare the absorption readings with those obtained with pure aqueous standards.

A Perkin Elmer atomic absorption spectrometer, Model 303, was used and a P.E. hollow cathode lamp 303-6040 served as a monochromatic light source. The flame was furnished by a three slot air acetylene burner. The lithium content was determined from the absorption at 670.8 nm. Lithium standard solutions were prepared from analytical grade Li\(_2\)CO\(_3\) (BDH).

REFERENCE:

SPECTROCHEMICAL ANALYSES OF ARCHEOLOGICAL MATERIALS*

I. Schoenfeld

Archeological samples were analyzed by means of emission spectrosopy because of the small amounts of material available for the determination of many elements (some in trace concentration). The speed and acceptable cost of spectrochemical analyses were also taken into account.

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*This work was carried out for the Israel Museum, Jerusalem
The simple technique using one standard in connection with a stepped filter was applied. The single standards (one for major, one for minor and one for trace elements) were prepared by dissolving metallic copper powder (Johnson-Matthey specpure) and adding adequate amounts of the elements to be determined. A sample of several milligrams was taken from an archeological object, and dissolved in nitric and hydrochloric acids. After addition of an adequate amount of specpure graphite, the solution was evaporated to dryness, ground and taken for excitation.

The spectra of samples and standards were recorded for 45 sec on the Jarrell-Ash grating spectrograph and the intensities of analytical and comparison lines were measured with the Jarrell-Ash microphotometer using, for each line, the most suitable filter step. The concentration was evaluated according to the formula:

\[ C_x = (1.44)^{n-1} C_s \left( \frac{I_x}{I_s} \right) \]  

where

- \( C_x \) and \( C_s \) are the concentrations of the sample and standard, respectively;
- \( I_x \) and \( I_s \) are the intensities of the analytical lines of the sample and standard, respectively
- \( n \) is the number of the filter step
- 1.44 is the experimentally established step factor

In Table 1 the spectral lines used and the composition of one sample are given as an example.

<table>
<thead>
<tr>
<th>Element</th>
<th>Wavelength of spectral line used (in ( \lambda ))</th>
<th>Concentration in %</th>
<th>Relative standard deviation % (Ref. 2)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Analytical line</td>
<td>Comparison line</td>
<td></td>
</tr>
<tr>
<td>Cu</td>
<td>CuI 2492.15</td>
<td>Background</td>
<td>82.70</td>
</tr>
<tr>
<td>Sn</td>
<td>SnI 2421.70</td>
<td>CuI 2441.64</td>
<td>9.50</td>
</tr>
<tr>
<td>Zn</td>
<td>ZnI 3282.33</td>
<td>CuI 3282.72</td>
<td>3.80</td>
</tr>
<tr>
<td>Fe</td>
<td>FeI 3091.58</td>
<td>CuI 3088.13</td>
<td>1.00</td>
</tr>
<tr>
<td>Pb</td>
<td>PbI 2801.99</td>
<td>CuI 3088.13</td>
<td>0.33</td>
</tr>
<tr>
<td>Cr</td>
<td>CrI 2731.91</td>
<td>CuI 2492.15</td>
<td>0.29</td>
</tr>
<tr>
<td>Ni</td>
<td>NiI 3050.82</td>
<td>CuI 3093.99</td>
<td>0.16</td>
</tr>
<tr>
<td>As</td>
<td>AsI 2780.22</td>
<td>CuI 3088.13</td>
<td>0.14</td>
</tr>
<tr>
<td>Ag</td>
<td>AgI 3382.89</td>
<td>Background</td>
<td>0.12</td>
</tr>
<tr>
<td>Sb</td>
<td>SbI 2311.47</td>
<td>CuI 2319.56</td>
<td>0.047</td>
</tr>
<tr>
<td>Mg</td>
<td>MgI 2776.69</td>
<td>CuI 3088.13</td>
<td>0.034</td>
</tr>
<tr>
<td>Bi</td>
<td>BiI 3067.72</td>
<td>CuI 3088.13</td>
<td>0.015</td>
</tr>
</tbody>
</table>
Cu and Sn were determined after a 100-fold dilution of the sample with graphite, Zn and Fe after a 10-fold dilution, and the other elements, present at concentrations below 1%, after a 2-fold dilution. Al and Si were also detected, but not quantitatively determined, since they may be present as common impurities.

The method revealed differences in the qualitative and quantitative composition of several samples.

REFERENCES:

DETERMINATION OF CARBON IN THIN LAYERS OF SILICON CARBIDE
R. Levin and N. Mayo

Chemical vapor deposition of various organic silanes over a silicon substrate in an atmosphere of H₂ or He between 850°C and 1350°C leads to the formation of thin films which contain mostly SiC. The SiC deposits may be contaminated with metallic silicon or free carbon.

A method is proposed for the determination of free carbon and silicon carbide carbon in these thin layers. One pre-weighing of the sample is required. The free carbon is determined by combustion of the sample at 800°C in a stream of oxygen. The carbon dioxide evolved is absorbed in 0.02N barium hydroxide solution and the excess is titrated with 0.01N potassium hydrogen phthalate solution. At this stage the SiC is not decomposed.

After cooling the combustion boat, the sample is covered with flux (2PbO.B₂O₃) and the carbidic carbon oxidized at 1000°C. The carbon dioxide evolved is determined as above. The combustion is completed in 15 minutes.

As little as 30 µg of carbon can be determined with sufficient accuracy.

REFERENCE:
HEALTH PHYSICS
The possibility of establishing a quantitative relationship between fast neutron dose and specific activation products in living tissue was explored. Such a relationship may be useful for fast neutron dose evaluation in routine neutron therapy and following accidental neutron over-exposures.

Tissue equivalent phantoms of different dimensions were exposed to 15 MeV D-T neutrons from a linear ion accelerator. One of the experimental arrangements is illustrated in Fig. 1. A polyethylene cylinder 27 cm in diameter and 43 cm high filled with tissue equivalent liquid was exposed to the neutron beam. Five inner bottles (numbered 1-5) filled with the same liquid were used to sample and measure activation products in the liquid after irradiation. Sets of activation samples (6, 7, 8, 9), containing various materials, were used to measure the thermal and fast neutron fluence. The phantom was replaced by an Anderson-Braun type neutron Rem-counter in order to estimate the dose equivalent from a direct measurement.
The radioactivity of activation products, such as from the reactions $^{14}\text{N}(n,2n)^{13}\text{N}$, $^{31}\text{P}(n,\alpha)^{28}\text{Al}$, $^{48}\text{Ca}(n,\gamma)^{49}\text{Ca}$ and $^{37}\text{Cl}(n,\gamma)^{38}\text{Cl}$ were measured immediately after irradiation by a whole body counter with a sensitivity of the order of 1 nCi. The neutron dose and its depth distribution were calculated\(^{(2,3)}\) and correlated with the activity of some of the activation products.

Assuming a delay of ten minutes between the end of irradiation and the start of counting, our results indicated that an activity of about 40 nCi $^{13}\text{U}/\text{Rem}$ and 60 nCi $^{38}\text{Cl}/\text{Rem}$ are available for measurement (activity per mean dose equivalent).

These results demonstrate the possible use of whole body counters or even simpler devices, e.g. shadow-shielded detectors, as routine instruments for dosimetry in fast neutron therapy.

REFERENCES:

CALIBRATION OF A DIRECT READING SOLID STATE DOSIMETER IN RADIATION THERAPY\(^{(1)}\)
V. Benary*, S.S. Friedland*, T. Schlesinger and A. Werner**

A small plane parallel lithium-drifted silicon p-i-n junction dosimeter mounted in a 3 mm diam, stainless steel tube with a 4 mil wall thickness was calibrated for use as an in vivo dosimeter to find the dose in the rectum after insertion of $^{137}\text{Cs}$ needles for cervix therapy.

The linear response of the dosimeter in the range of interest, its wavelength dependence, and the intercomparison with TLD dosimeters, both in calibration and clinical use, and the dependence of the rectal dose on the position of the applicators in the uterus, were studied.

For calibration purposes, a block of lucite was used as a phantom. Holes were drilled into the lucite, one for a $^{137}\text{Cs}$ tube (20 mg radium equivalent) and 10 others for the detector at distances of 1 to 10 cm from

*Tel-Aviv University, Ramat Aviv
**Sheba Medical Center, Ramat Gan
the source. The depth of the holes was such that the detector was always along the midline of the applicator. The absorbed dose rate was calculated for the 10 detector locations assuming the source to be a point source and taking the spacial dependence in air as $1/r^2$. Corrections for absorption and buildup were made. To verify the above calculations and assumptions, a number of TLD dosimeters were irradiated in the same geometry and read out. The TLD dosimeters were replaced by a silicon detector and a curve of counts per second as a function of position was obtained. The discrimination level was such that the background was zero both at room and body temperatures.

Dose rates obtained from calculated data (Fig. 2) and those measured by the TLD dosimeters (Fig. 3) are plotted against the count rate obtained with the silicon detector. A good agreement between the two calibration curves is evident.

REFERENCE:
DOSE DISTRIBUTIONS IN TANGENTIAL IRRADIATION OF THE CHEST WALL

M. Israeli, T. Schlesinger, Y. Klopf er, M. Tat cher and Y. Cohen

Following mastectomy in breast cancer patients, radiation therapy is
often given to destroy residual tumor cells within the surgical field and in
the related lymph nodes. A wide variety of radiation techniques have been
utilized for this purpose. The dose distributions obtained when the chest wall
is irradiated by cobalt-60 tangential fields (45° wedged fields with a 2.5 mm
thick rubber sheet bolus) were studied.

The dose distributions were calculated by manual and computer methods.
Body curvature was taken into account in the manual calculations by the
isodose shift method and in the computer calculations by applying an absorption
correction. The corresponding doses were measured in pressed wood phantoms,
shown in Fig. 4, with Harshaw TLD-100 detectors in the form of 3x3x1 mm³
ribbons for internal points and 3x3x0.3 mm³ ribbons for surface points.

Fig. 4
Phantom contour for chest wall irradiation
(tangential fields)

*Rambam University Hospital, Haifa
In Fig. 5 calculated and measured dose distributions for wedged fields with bolus are compared. The solid lines indicate the calculated values while the circled numbers give the results of the measurements inside the phantom.

![Diagram of dose distributions for wedged fields and bolus](image)

**Fig. 5**

*Calculated and measured dose distributions for wedged fields and just under the bolus. Normalization has been applied so that 100 corresponds to the given dose. It is evident that there is good agreement between the measured and calculated doses and that the skin dose is continuous with the internal dose.*

The thin TLD detectors were used to give an approximation of the skin dose, i.e. the dose between depth 0 and 0.3 mm, in the absence of the bolus. For the above case the readings of detectors placed on the irradiated surface were from about 60% to 70% of the mean target dose.

As a result of calculations and measurements for contours of various shapes, it is concluded that a tangential cobalt technique with wedges and bolus can provide a good dose distribution in the chest wall for most patients.

**REFERENCE:**

EFFECTS OF HEMATOPORPHYRIN ON PHOTOPRODUCTS FORMATION IN UV-IRRADIATED THYMINE

E. Riklis, A. Prager and E. Elhanani

Porphyrins tend to localize in certain human and animal tumors. It has been reported that X-ray therapy in conjunction with various injected porphyrins resulted in significant response, and that hematoporphyrins greatly increase the X-radiation sensitivity of paramecia. Bearing in mind that thymine dimers, which are responsible for cell damage following UV-irradiation, are also responsible for tumor production in certain organs, the effects of porphyrins on thymine dimer production were studied. It was found that the addition of hematoporphyrin sensitizes a frozen solution of thymine. UV-irradiation of methyl-3H-thymine frozen solution and separation of photoproducts by radiochromatography resulted in a 3-5 fold increase in production of thymine dimers as well as in the appearance of another yet unidentified photoproduct. This sensitization is pH and concentration dependent, with a maximum effect shown by 1x10^{-5} M hematoporphyrin with 1x10^{-4} M thymine. The effect on DNA and on whole cells is under study.

REFERENCE:

DISTRIBUTION AND CLEARANCE STUDIES OF CHELATED 169Yb AND 99mTc IN LOCALLY PRODUCED PHARMACEUTICALS - A PRELIMINARY REPORT
A. Naharin and J. Trumper

In radiobiological assay, in-vivo tests of chelated radiopharmaceuticals are becoming an increasingly essential part of quality control and a reliable means of evaluating production methods. It is important to know if local production processes of radiopharmaceuticals and kits supplied to hospitals are properly maintained and are comparable to those of similar laboratories as to the quality and efficacy of the preparations.

Doses between 0.2-1.0 mCi/0.2 ml were intravenously injected into ICR mice of local strain. Distribution measurements were carried out on several organs and tissues of importance at various time intervals after administration. Blood and skeletal uptake were calculated by extrapolation from fractional samples. All measurements were done by means of a single channel analyzer. A 3" NaI well crystal was used in distribution measurements and a whole-body counting system made up of 5" and 3" NaI crystals was used for clearance measurements.

Table 1 gives the results obtained for several common locally produced
### Table 1

Distribution of radiopharmaceuticals in various organs and tissues of the mouse at different times after dose administration

<table>
<thead>
<tr>
<th>Drug</th>
<th>Target organ(s)</th>
<th>Time after injection (min)</th>
<th>% of Body Burden</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Blood</td>
</tr>
<tr>
<td><strong>99m</strong>Tc-Sulfur colloid (SC)</td>
<td>Liver</td>
<td>15</td>
<td>5.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
<td>3.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>45</td>
<td>6.4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>60</td>
<td>6.5</td>
</tr>
<tr>
<td><strong>99m</strong>Tc-Macro aggregate albumin (MAA)</td>
<td>Lungs</td>
<td>15</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>60</td>
<td>0.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>120</td>
<td>0.1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>240</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>24 h</td>
<td>0.5</td>
</tr>
<tr>
<td><strong>99m</strong>Tc-Diethylene diamine pentaacetic (DTPA)</td>
<td>Kidneys, bladder</td>
<td>15</td>
<td>18.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
<td>7.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td>60</td>
<td>2.1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>120</td>
<td>1.2</td>
</tr>
<tr>
<td><strong>99m</strong>Tc-Fe-ascorbic acid</td>
<td>Kidneys</td>
<td>60</td>
<td>4.8</td>
</tr>
<tr>
<td><strong>99m</strong>Tc-EHDP</td>
<td>Skeleton</td>
<td>120</td>
<td>1.0</td>
</tr>
<tr>
<td><strong>99m</strong>Tc-Tetracycline</td>
<td>Liver, kidneys, heart</td>
<td>15</td>
<td>18.3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30</td>
<td>5.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>60</td>
<td>4.3</td>
</tr>
<tr>
<td><strong>99m</strong>Tc-Human serum albumin</td>
<td>Blood</td>
<td>60</td>
<td>19.4</td>
</tr>
<tr>
<td><strong>75</strong>Se-methionine</td>
<td>Pancreas</td>
<td>60</td>
<td>6.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td>120</td>
<td>4.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>180</td>
<td>5.7</td>
</tr>
<tr>
<td><strong>189</strong>Gold colloid</td>
<td>Liver</td>
<td>24 h</td>
<td>3.0</td>
</tr>
</tbody>
</table>
radiopharmaceuticals in various target organs and at different times after dose administration. Further comparison studies will be undertaken.

DECONTAMINATION EFFICIENCY OF DTPA COMPLEX WITH $^{169}$Yb BY VARIOUS ROUTES OF ADMINISTRATION - PRELIMINARY EXPERIMENTS
A. Naharin

When a heavy rare-earth metal is chelated to diethylenetriamine-pentaacetic acid (DTPA) and administered into the body, it is quickly eliminated via the kidneys\(^\text{(1)}\) (99\% during the first 24 hours). This is not the case when DTPA is injected after the contaminant is already incorporated or when the chelation occurs within the body. The efficiency of DTPA as a clearing agent is then reduced inversely according to the time lapse between the contamination and DTPA administration\(^\text{(2,3)}\). The rapid disappearance from the blood of DTPA, although very convenient for diagnostic purposes, is less desirable when the DTPA is needed for decontamination. The chelation of the contaminant with DTPA might be made more efficient if the presence of DTPA in the circulatory system could be prolonged. The aim of this work was to find if this prolongation would come about if DTPA were not administered intravenously but via one of the other parenteral routes.

Four out of five female ICR mice in four experimental groups were given a dose of 3 $\mu$Ci/0.2 ml $^{169}$YbCl\(_3\) as a tracer; the fifth was used as a control for external contamination. Within each experimental group four routes of administration were used - intravenous (IV), intraperitoneal (IP), intramuscular (IM) and subcutaneous (SC). Table 2 gives the body burden of Yb-DTPA at different times after administration. It can be seen that, in general, the speed of clearance via the four routes followed the order: intravenous, intramuscular, intraperitoneal and subcutaneous. It can also be seen that the clearance in group 2, where the contaminant was injected chelated to DTPA, was quickest for all four routes of administration.

Thus, the assumption that the introduction of the DTPA via a slower route would increase the rate of clearance of contaminant was not verified.

REFERENCES:
# TABLE 2

The body burden of ytterbium chelated to DTPA administered to mice via various routes and at different times after injection

<table>
<thead>
<tr>
<th>Exp. group</th>
<th>Route of administration</th>
<th>% of dose at various times after administration</th>
<th>3 h</th>
<th>6 h</th>
<th>24 h</th>
<th>48 h</th>
<th>4 days</th>
<th>7 days</th>
<th>14 days</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>93.7± 7.6</td>
<td>91.5± 14.5</td>
<td>94.0± 6.4</td>
<td>82.0± 3.2</td>
<td>93.7± 4.0</td>
<td>14.7± 2.5</td>
<td>24.3± 3.4</td>
</tr>
<tr>
<td>1. Control-YbCl$_3$ only</td>
<td>SC</td>
<td></td>
<td>88.2± 8.2</td>
<td>87.4± 13.6</td>
<td>92.9± 7.0</td>
<td>73.0± 5.0</td>
<td>86.2± 7.6</td>
<td>92.9± 7.0</td>
<td>92.2± 7.6</td>
</tr>
<tr>
<td></td>
<td>IM</td>
<td></td>
<td>76.2± 11.3</td>
<td>75.3± 13.5</td>
<td>86.2± 7.6</td>
<td>67.1± 5.0</td>
<td>81.8± 8.3</td>
<td>86.2± 7.6</td>
<td>81.8± 8.3</td>
</tr>
<tr>
<td></td>
<td>IP</td>
<td></td>
<td>73.0± 5.0</td>
<td>71.4± 12.7</td>
<td>64.0± 4.9</td>
<td>61.5± 5.2</td>
<td>76.0± 8.6</td>
<td>76.0± 8.6</td>
<td>76.0± 8.6</td>
</tr>
<tr>
<td></td>
<td>IV</td>
<td></td>
<td>70.5± 4.0</td>
<td>67.4± 14.3</td>
<td>61.5± 5.2</td>
<td>57.2± 3.8</td>
<td>86.6± 9.3</td>
<td>86.6± 9.3</td>
<td>86.6± 9.3</td>
</tr>
<tr>
<td>2. Yb-DTPA complex</td>
<td>SC</td>
<td></td>
<td>28.9± 5.2</td>
<td>14.7± 2.5</td>
<td>9.8± 0.9</td>
<td>9.8± 0.9</td>
<td>9.8± 0.9</td>
<td>9.8± 0.9</td>
<td>9.8± 0.9</td>
</tr>
<tr>
<td></td>
<td>IM</td>
<td></td>
<td>12.4± 2.2</td>
<td>2.6± 0.6</td>
<td>1.2± 0.1</td>
<td>1.2± 0.1</td>
<td>1.2± 0.1</td>
<td>1.2± 0.1</td>
<td>1.2± 0.1</td>
</tr>
<tr>
<td></td>
<td>IP</td>
<td></td>
<td>2.1± 1.6</td>
<td>1.6± 0.1</td>
<td>0.9± 0.3</td>
<td>0.9± 0.3</td>
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<td>0.9± 0.3</td>
</tr>
<tr>
<td></td>
<td>IV</td>
<td></td>
<td>1.2± 1.0</td>
<td>1.0± 0.1</td>
<td>0.9± 0.3</td>
<td>0.9± 0.3</td>
<td>0.9± 0.3</td>
<td>0.9± 0.3</td>
<td>0.9± 0.3</td>
</tr>
<tr>
<td>3. YbCl$_3$ (IV) &amp; DTPA</td>
<td>SC</td>
<td></td>
<td>64.3± 3.3</td>
<td>59.5± 4.8</td>
<td>58.0± 5.6</td>
<td>55.5± 5.8</td>
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<td>55.5± 5.8</td>
<td>55.5± 5.8</td>
</tr>
<tr>
<td></td>
<td>IM</td>
<td></td>
<td>59.5± 4.8</td>
<td>58.0± 5.6</td>
<td>55.5± 5.8</td>
<td>55.5± 5.8</td>
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<td>55.5± 5.8</td>
<td>55.5± 5.8</td>
</tr>
<tr>
<td></td>
<td>IP</td>
<td></td>
<td>63.4± 5.8</td>
<td>58.0± 5.1</td>
<td>55.4± 4.4</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>4. YbCl$_3$ (IV) &amp; DTPA</td>
<td>SC</td>
<td></td>
<td>47.3± 4.0</td>
<td>43.8± 5.2</td>
<td>43.8± 4.1</td>
<td>41.5± 4.7</td>
<td>41.5± 4.7</td>
<td>41.5± 4.7</td>
<td>41.5± 4.7</td>
</tr>
<tr>
<td>15 min later</td>
<td>IM</td>
<td></td>
<td>47.3± 4.0</td>
<td>43.8± 5.2</td>
<td>43.8± 4.1</td>
<td>41.5± 4.7</td>
<td>41.5± 4.7</td>
<td>41.5± 4.7</td>
<td>41.5± 4.7</td>
</tr>
<tr>
<td></td>
<td>IP</td>
<td></td>
<td>43.0± 3.9</td>
<td>39.5± 3.0</td>
<td>37.0± 3.3</td>
<td>36.6± 3.0</td>
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<td>36.6± 3.0</td>
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</tr>
<tr>
<td></td>
<td>IV</td>
<td></td>
<td>21.6± 2.3</td>
<td>21.1± 2.0</td>
<td>19.0± 3.1</td>
<td>18.0± 3.0</td>
<td>18.0± 3.0</td>
<td>18.0± 3.0</td>
<td>18.0± 3.0</td>
</tr>
</tbody>
</table>

*The 15-minute time gap was chosen to simulate conditions of accidental contamination in a laboratory.
RADIATION INDUCED ORGANOGENESIS IN TOBACCO TISSUE CULTURE

N. Degani

The formation of leafy buds in dark-grown tobacco tissue culture ("Nicotiana tabacum" var. Wisconsin no. 38) was induced by irradiation. Organ formation was also induced indirectly, by culturing non-irradiated tissue on an irradiated medium. Experiments were designed to determine which component of the medium was effective in the induction of organ formation. Fractions of the growth medium were irradiated singly and combined with non-irradiated fractions.

The results showed that formation of leafy buds was not concomitant with the irradiation of IAA. Omission of IAA from a non-irradiated medium induced differentiation as expected. Irradiated myo-inositol, under certain experimental conditions, induced organogenesis more consistently than the other irradiated components.

The age of the inoculum tissue and its passage number from the original tobacco stem determined its ability to form organs. In most experiments, cultures which were extracted from a stock younger than 45-50 days did not differentiate. The control mechanism for differentiation deteriorated after about 13 passages, after which the cultures differentiated in the darkness even on a non-irradiated medium.

REFERENCE:

NITRITE-INDUCED DEVELOPMENT OF THE NITRATE UPTAKE SYSTEM IN PLANT CELLS

Y.M. Heimer

Nitrate is known to induce the development of the nitrate uptake system and the nitrate and nitrite reductase activity in XD cells of tobacco (1-3) and other plants (4,5). In some plants (3,6) nitrite can be substituted for nitrate to induce nitrate and nitrite reductase activities. Lips et al. (6) suggested recently that in pea cotyledons, nitrite, and not nitrate, is the true direct inducer of the two enzymes. The present work was carried out to determine whether nitrite can induce the nitrate uptake system in XD cells.

Cells of the XD line of tobacco were grown as previously described (1,2) to the mid-logarithmic phase, harvested and resuspended in a nitrogen-free medium, one part being supplemented with 3.0 mM KNO₃ and another part with 0.5 mM KNO₂. After incubation for 5 hours, all of the cells were given
enough KNO₃ to bring the nitrate concentration of the medium to 10.0 mM. At certain time intervals, aliquots of the cell suspensions were removed and the nitrate reductase activity (a) and the nitrate content (b) of the cells were determined, as shown in Fig. 6.

![Graph showing nitrate reductase activity and nitrate content over time](image)

**Fig. 6**
Development of nitrate reductase activity (a) and accumulation of nitrate (b)
- 3.0 mM KNO₃; o 0.5 mM KNO₂

As expected (3,5), cells induced with either nitrate or nitrite developed nitrate reductase activity. The activity developed more rapidly and to a higher level in cells induced with nitrite than in cells induced with nitrate. This higher activity declined subsequently, to a level which was similar to that in cells induced with nitrate. Nitrate accumulation by cells induced with nitrate started at a low initial rate of 0.3 μmoles of nitrate accumulated/h/g fresh weight. The rate of accumulation increased to a constant value of 1.0-1.5 μmoles accumulated/h/g fresh weight, by the 2nd hour. During the first hour after the addition of nitrate to the medium (between the 5th and the 6th hours), nitrite-induced cells accumulated about 4 μmoles of nitrate/g fresh weight. This amount of nitrate taken up by nitrite-induced cells is 10-fold higher than the amount taken up during the first hour by cells induced with nitrate. The subsequent rate of accumulation by nitrite-induced cells was lower than the initial rate. This was expected since nitrite inhibits nitrate accumulation (1).

A low initial rate of nitrate accumulation, increasing with time to a constant value, was interpreted (1) as an indication that the uptake system was induced by the addition of nitrate. A high initial rate of accumulation as compared with controls would indicate that the uptake system was already
induced at the time of the addition of nitrate. In the experiment described here, a low initial rate of nitrate accumulation by cells not induced by nitrite and a high initial rate of accumulation by cells induced with nitrite were observed.

It is concluded that the uptake system was induced by the nitrite and was, therefore, fully operative when the nitrate was added to the medium. Thus, nitrite can be a substitute for nitrate as an inducer not only of the nitrate and nitrite reductase activities (2–5), but also as an inducer of the entire assimilation pathway. This is a case where an intermediate product of a particular pathway induces the development of the uptake system of that pathway.

REFERENCES:
ENVIRONMENTAL STUDIES
ANALYTICAL EXPRESSION FOR THE VERTICAL DISPERSION COEFFICIENT

D. Skibin

To estimate the concentration of dispersed air pollution, the lateral and the vertical dispersion coefficients $\sigma_y$ and $\sigma_z$ have to be determined. These coefficients are functions of atmospheric stability and of the distance downwind from the source.

Analytical expressions for the dispersion coefficients were derived by Tadmor and Gur\(^{(1)}\). The expression for $\sigma_y$ presented no problem since the Pasquill-Gifford\(^{(2-4)}\) curves for $\sigma_y$ are straight lines on the log $\sigma_y$ - log $x$ plot. The fact that the $\sigma_z$ curves are much more complicated led Tadmor and Gur\(^{(1)}\) to approximate the curves by straight lines (on log-log paper) in two separate zones, i.e. 0-5 and 5-50 km downwind distance. Expressions for distances over 50 km were not given.

In order to use the Pasquill-Gifford system for numerical calculations, Imai and Iijima\(^{(5)}\) used the following form for $\sigma_y$ and $\sigma_z$:

\[
\sigma_y = K_0 x (8 - \log x) \quad (1)
\]

\[
\sigma_z = \sigma_0 x^{a_1 x + a_2 x^2} \quad (2)
\]

Using the least squares method the different parameters were determined by Imai and Iijima\(^{(5)}\). A careful examination of the Pasquill-Gifford curves shows that the suggested analytical expressions do not, a priori, fit the curves, though almost any line can be approximated by a polynomial or even a more complex function of $x$.

The present work leads to the conclusion that Pasquill-Gifford's $\sigma_z$ curves should be represented as an exponential function of log $\sigma_z$ in which the variable is log $x$.

The numerical values of the parameters of this function were computed and presented for each stability category. The results fit the $\sigma_z$ curves over the whole range of $x$, up to 100 km downwind distance.

REFERENCES:
VARIATION OF LATERAL GUSTINESS WITH WIND SPEED

D. Skibin

The variation of lateral gustiness with wind speed was studied using a light-weight, fast response wind system coupled to an automatic sampling and multichannel analyzer set-up. Accuracies of 1° in determining the width of wind direction distribution and 1 km/h in determining wind speeds above the 1 km/h threshold were obtained.

Results support a decreasing trend in lateral direction fluctuations with wind speed, for speeds over 2 m/sec. For light winds up to 2 m/sec, direction fluctuations increase wind speed, during both stable and unstable conditions.

It is suggested that increasing wind speed is necessary to provide the energy to overcome pressure resistance to lateral fluctuations which therefore increase with wind speed. This result is consistent with continuity considerations. At higher wind speeds, increasing air momentum results in a decrease in fluctuations with increasing wind speed. The product of wind speed and width of lateral fluctuations increases monotonically for all wind speeds, which agrees with present experimental evidence.

REFERENCES:

3-DIMENSIONAL ANALYSIS OF THE WIND FLOW PATTERN IN THE SOUTHEASTERN PART OF ISRAEL

D. Skibin

A study of the synoptic situation in the south-eastern part of Israel led to the conclusion that the dominant feature is a pressure ridge extending from south to north over the main Israeli mountain ridge. This pressure ridge results mainly from regional influences. It causes a partial separation of the flow systems, air masses, and climates on its north-western and south-eastern sides.
Measurements of wind direction and speed for the summer months in stations on the mountain ridge and down in the Arava support the above conclusion. The separation of flow is so pronounced that the measurements indicate the existence of a land-sea breeze system around the Dead Sea, during periods in which the main Mediterranean breeze system does not override it.

**THE OFFSHORE BARS AT ASHDOD: TOPOGRAPHY, SEASONAL BEHAVIOR AND "INDICATIVE RATIOS"**

H.L. Striem

In planning coastal installations, such as those needed to regulate the intake and discharge of cooling water for a nuclear power plant, the topography and behavior of the offshore bars should be considered.

Along Israel's sandy southern Mediterranean coast, there is usually one main offshore submarine bar. It was found that the bars are not monotonous ridges, but recurrent structures of a significant topography: broad and shallow parts lying nearest the shore, and narrowing branches increasing in depth and distance from the shore. The broad "trunk" sections are linked to the inshore by a regularly recurring submarine spur or a saddle structure. The trough, separating the bar from the inshore, widens as the bar narrows, and enlarges into a deep basin near the sill, the deepest and narrowest section of the bar ridge.

The bars usually have skew profiles, reflecting their seasonal movement. During summer and under low waves the bars approach the shore due to a drift-like sediment movement, and they recede seawards after severe storms, as occur during winter, due to a return flow across the bar. The topographic structure interacts with the local flow pattern, the trough channelling the longshore flow which is discharged seawards over the sill as a rip current.

It was also found that the ratios between certain bar parameters are indicative of the geomorphic condition of the bar. Thus the ratio of the depth of the trough to the depth of the crest may reach and exceed 1.7 when the first winter storms arrest the shoreward movement of sediment. The ratio drops to 1.2 when the bar has been flattened seawards. The ratio of the distance of the crest from the shore to the depth of the crest is also indicative, reaching 80 and more at the end of winter and decreasing to about 55 during the summer when the bar approaches the shore.
CONCENTRATION DYNAMICS INVESTIGATIONS IN LARGE SCALE OXIDATION PONDS
I. Frenkel, Ch. Gilath, M. Meltzer, I. Frydman * and A. Levin

The concentration dynamics of inert soluble matter was investigated on one of the oxidation ponds of the Dan Region Sewage Reclamation Project. The pond is relatively shallow (2-2.5 m depth), has a volume of about 150,000 m$^3$ and a mean residence time of about 6 days.

Two experiments were performed with $^{82}$Br (KBr in solution) as tracer. The tracer was injected in the inlet channel and its activity measured at different outlets and also in the pond (from a boat). The first experiment involved an activity of 72 mCi and lasted for 96 hours. The activity injected in the second experiment was 3.3 Ci and measurements lasted for 10 days. Both experiments proved that the pond is well mixed by wind-induced currents. However, under special conditions of wind direction, strong currents towards the outlet of the pond were found to be responsible for a certain amount of short circuiting. It was proven that a good knowledge of the wind statistics and a few current measurements (using drogues) plus a tracer experiment of short duration are sufficient for a fairly good understanding and modelling of the concentration dynamics of inert soluble matter in the pond.

USE OF GASEOUS TRACERS IN THE ATMOSPHERE FOR MONITORING AND CONTROL OF AIR POLLUTION IN URBAN AREAS

J. Binenboym, I. Gilath, Ch. Gilath, M. Meltzer, M. Rinsberger ** and A. Manes **

The aims of this newly initiated project are: a) to determine the contribution of a particular pollutant source to the overall pollution level in the urban areas of Israel, b) to test different dispersion models and determine the dispersion coefficients in the urban areas, c) to determine the rate of disappearance of certain pollutants in the atmosphere.

Several pollutant sources exist, the greatest being power plants which give off SO$_2$. This work will permit obtaining information on the contribution of each of these plants to the overall pollution level to establish the dispersion pattern and disappearance of pollutants from the area by means of an easy and inexpensive technique involving the use of an inert tracer, such as SF$_6$.

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* This work was performed for Mekoroth Water Co. Ltd.
** Israel Meteorological Service, Beit Dagan
*IAEA fellow from Federal University of Rio Grande do Sul, Porto Alegre, R.G., Brazil.
++ This work is partly supported by the National Council for Research and Development
Sulfur hexafluoride, as well as other halogenated compounds, have proven to be useful tracers of many varieties of air masses, e.g. the detection of surface air masses and tracing of stack effluents both on the ground and in the air. SF$_6$ is most useful as a tracer because of its ultrasensitive detection by electron capture chromatography (0.1% SF$_6$ in air), chemical stability in the presence of other atmospheric pollutants and sunlight, and normally negligible concentrations in the atmosphere.
INSTRUMENTATION AND TECHNIQUES
FIRST TRIAL OPERATION OF THE MEIRA ELECTROMAGNETIC ISOTOPE SEPARATOR
I. Chavet, M. Kanter and H. Menat

The MEIRA separator has been described previously\(^1,2\). The first source installed was of the calutron type with internal cathode. For the first trial runs, it was operated mainly with nitrogen. The source was tried with current regulation both in the cathode limited mode and pressure limited mode with satisfactory results up to its maximum arc current of 15 A.

When the high voltage was applied, difficulties with beam neutralization and very frequent sparking were encountered. The reason was found to be a faulty design of the extraction electrode. Being too narrow, it could not sufficiently shield the beam from the influence of the extraction field overflowing the sides of the electrode. Widening the electrode completely eliminated neutralization problems and reduced sparking significantly. It is planned to increase the source magnetic field gap in order to reduce the sparking between the source and the poles of the source magnet still further.

The beam crossing in the axial plane at the magnet entrance, which is one of the main features of MEIRA optics, was very satisfactory, namely the cross-over in the Z-direction was less than 1 cm for a source slit of 10 cm. However, ions emitted near the edges of the slit do not follow trajectories which can be easily controlled. Various methods are being tested to effectively control these edge effects.

The acceleration system was tested with electrode profiles according to the calculated Pierce curves\(^3\) and found to yield a much higher beam divergence than the theoretical one. The emission electrode was then replaced provisionally by the more common electrode with an aperture angle of 120° for resuming source trials. A first calculation\(^4\) indicated that the lens effect of the electrode slit may well be the factor responsible for the increased divergence.

The source was tried under high voltage and stable beams of nitrogen up to 95 mA (measured at the source) were obtained. However, the optical quality of the image could not be tested because of difficulties encountered in the regulation of the high voltage.

The main problems are a significant residual ripple in the output and an intolerable sensitivity of the electronic components to high voltage surges.
caused by electrode sparking. Work is being pursued to overcome these difficulties.

REFERENCES:
4. Menat, M., Chavet, I., and Kantor, M., this annual report, see below.

THE LENS EFFECT OF THE HOLE OR SLIT IN THE EXTRACTION ELECTRODE OF HIGH CURRENT ION SOURCES

M. Menat, I. Chavet and M. Kantor

During the trial runs of the electromagnetic isotope separator MEIRA it was found that an electrode system shaped to the theoretical Pierce profiles gave a beam divergence much higher than the calculated value.

The lens effect of the electrode slit was suspected of contributing significantly to the increased divergence. Although expressions are known to describe this effect, they are valid only for space charge free configurations. Relying on some simplifying assumptions, the lens effect of the slit or hole in the extraction electrode was calculated for the case of high intensity ion beams where space charge cannot be neglected.

For the case of a slit, the divergence increment due to the lens effect is roughly:

$$\Delta \alpha \sim \frac{1}{2} (\alpha + \beta) \left[1 + \frac{4}{5} \frac{\alpha}{\beta} \right]$$

where $\alpha$ is the initial beam divergence determined by the meniscus curvature and $\beta$ is the angle through which the meniscus width is seen from the center of the electrode slit (Fig. 1).

For the case of a hole, one obtains, with the same notation:

$$\Delta \alpha \sim \frac{1}{4} (\alpha + \beta) \left[1 + \beta \left(1 + \frac{\alpha}{\beta}\right)^{0.63} \right]$$
KANDI III - A TRIPLE AXIS NEUTRON SPECTROMETER
M. Melamud and H. Shaked

The KANDI III spectrometer (Fig. 2) was recently mounted on a radial beam hole in the IRR-2 and will be used for studying spin waves in antiferromagnetic crystals by inelastic neutron scattering.

The monochromator is a pyrolytic graphite crystal of \( \approx 30' \) mosaic spread, and the analyzer a bank of four pieces of pyrolytic graphite giving a mosaic of \( \approx 100' \). Four stepping motors drive the sample axis, analyzer arm, analyzer axis and counter arm. Angles are measured by means of absolute digitizers mounted directly in the shafts of the four stepping motors, giving a resolution of \( \approx 1/3 \) of a minute of arc for the axes and arms. The output from the digitizers is fed into an HP-2100 computer which controls the spectrometer "on-line". The computer translates points in energy-momentum \((E,q)\) space into four angles for the four motors, thus making possible any scan through \(E,q\) space.
As part of the testing of the equipment, phonons in copper were measured. The sample was a single crystal disc of copper, 5 cm in diameter, 0.6 cm thick. The results for the acoustic transverse branch in the [111] crystallographic direction are shown in Fig. 3. The insert shows a typical neutron group. The resulting dispersion curve is compared with the dispersion curve
Dispersion curve for copper in the symmetry direction [111] near the (220) reciprocal lattice point. The insert shows a typical neutron group obtained by the constant - q method given by Svensson et al. Our data are not corrected for the instrument resolution.

REFERENCE:

IMPROVEMENT OF MASS SPECTROMETRY TECHNIQUES
A. Cohen and Y. Zimmerman

The results of isotopic ratio measurements using mass spectrometry are normally presented as an analog record on a chart recorder. The usual treatment of these data requires measurements of peak heights while subtracting the corresponding noise factor. The reproducibility thus obtained is limited mainly by the statistical variation of the number of the collected ions and by the reference points chosen by the operator. The purpose of this work is to develop means and techniques that will improve the precision and reliability of such measurements.
The magnet current of the mass spectrometer is controlled automatically by a magnet current controller, by causing changes in the ion current "peaks" which are proportional to the relative amounts of the measured isotopes. In this system the current detected by an electron multiplier is amplified and fed into an analog-to-digital converter. Then it is recorded on tape by means of an incremental magnetic recorder.

Computer data processing permits either direct calculation of the areas under the peaks or comparison of their contours. From these areas the average mass ratio is obtained by a least squares calculation. In addition a comparison of contours of many corresponding peaks integrates their statistical fluctuations to zero. The ratio of the average peaks obtained in this way is the average mass ratio of the isotopes.

The system is now being run in. Some preliminary results of the isotope ratios of $^{185}\text{Re}/^{185}\text{Re},$ $^{235}\text{U}/^{238}\text{U}$ are in close agreement with their occurrence in nature.

RADIOACTIVE IONIZATION GAUGE
A. Berman

A radioactive ionization gauge using a $^3\text{H}$ target as ionizing source was developed. A linear relationship between the gauge output and equivalent densities of air in the range $10^{-1}$-$10^{-3}$ Torr was obtained by special design considerations. The outputs are accurate and remarkably reproducible. The gauge is not hazardous to personnel. Further work is being conducted to extend the range of measurement.

GRAPHICAL EVALUATION OF THE MERCURY VAPOR PUMPING EFFECT ON McLEOD GAUGE MEASUREMENTS
A. Berman

Pressure measurements with a McLeod gauge backed by a cold trap are erroneous because of the mercury vapor pumping effect. Errors altering McLeod gauge pressure readings were calculated. A large range of laboratory temperatures and of radii of connective tubing to the cold trap were taken into account. Dry $\text{N}_2$ was used as the calibration gas. The results were graphically expressed; see Fig. 4. Pressure readings taken on a commercial McLeod gauge and a capacitance manometer were compared in a calibration system. The experimental and calculated results are in good agreement.
Fig. 4

Variation of \( \Delta p/p_0 \) as a function of temperature for connective tubing radii ranging from 0.20 to 1.00 mm

REFERENCE:

OUTGASSING PROPERTIES OF PERSPEX
H. Galron

Information on the outgassing properties of Perspex was obtained using a magnetic mass spectrometer. The specimen, with a surface area of 280 cm\(^2\), was exposed to atmosphere before testing.

The total outgassing rate and that of specific component gases is given as a function of pumping time in Fig. 5. It is seen that water vapor is the main component and apparently covers the surface in such a way that it decreases
the outgassing rate of other gases. After a certain amount of water has been removed the outgassing of the other gases increases with pumping time.

ELECTROSTATIC AND FOIL ELECTRET MICROPHONES
P. Buchman

The properties of polyvinylidene fluoride (PVF$_2$) foil electret microphones (1) were investigated. The microphone has a sensitivity of -60 dBV/μbar in the frequency range of 20 Hz to 6 kHz. The signal output decreases, however, with time as a result of homocharges and heterocharges in the foil (2).

When operated as an electrostatic microphone the signal, in the form of a butterfly loop, depends on voltage to the third power. The sensitivity of the microphone, at a fixed bias, increases with temperature from -47 dBV/μbar
at 20°C to a maximum of -38 dBV/µbar at 90°C and then falls as a result of the changes in the elastic properties of the material.

REFERENCES:

SEEBECK COEFFICIENT OF THERMOELECTRIC MATERIALS
M. Lanxner and I. Shai

The Seebeck coefficient of a material is given by the limit of the voltage measured across the sample as the applied temperature difference approaches zero \(^{(1)}\). Hence, it is given by the gradient of potential per unit temperature gradient with the current equal to zero:

\[
\frac{dE}{dx} = -a \frac{dT}{dx}
\]

The variation with temperature and direction of the Seebeck coefficient is essential in thermoelectric materials research \(^{(2)}\). Such measurements were made on several thermoelectric samples. The heat block assembly is shown in Fig. 6a. The sample, S, is held between the spring loaded heat blocks H. The thermoelectric voltage is read from the copper leads of temperature measuring Cu-constantan thermocouples, (Fig. 6b). This ensures that both the temperature and the thermoelectric voltage are being measured at the same place \(^{(3)}\).

Fig. 6
Arrangement for Seebeck coefficient measurements
A high input impedance digital voltmeter is used to read the voltages of thermocouples and sample.

The Seebeck coefficient of a material such as Bi$_2$Te$_3$ is of the order of 200 µV/°C. Taking advantage of this, one can obtain the Seebeck coefficient for small temperature differences, such as 0.5°C.

Measurements of α covered the temperature range 20°C - 150°C and were made for the three directions of each cubic sample. Anisotropy of the thermoelectric power was clearly observed and values higher by 25-50 µV/°C in the best direction were obtained.

REFERENCES:

THERMAL CONDUCTIVITY OF THERMOELECTRIC MATERIALS
I. Shai and Y. Levi

In determining the best thermoelectric material for direct energy conversion, one comes up with a criterion called the figure of merit of the material \( Z = \alpha^2 / k \rho \), where \( k \) is the thermal conductivity and \( \alpha, \rho \) are the Seebeck coefficient and electrical resistivity, respectively. Thermoelectric materials are considered to be of low thermal conductivity and special techniques are required for measuring this property.

In this work an apparatus was built for absolute measurement of thermal conductivity of thermoelectric materials. A schematic drawing is given in Fig.7.
Two pieces of the same thermoelectric material oriented in the same direction are placed in series with 3 copper discs each of which is connected to a Cu-constantan thermocouple. The middle copper disc also contains an electrical resistor which acts as the heating source.

The temperature gradients in samples I and II (in the figure) are calculated in two ways: by direct measurement of the temperatures with the thermocouple and by measuring the electrical potentials across the blocks with the same copper thermocouple wires.

THE ELECTRICAL RESISTIVITY OF BISMUTH-TELLURIDE AT TEMPERATURES BETWEEN 25°-280°C
U. Admon and I. Shai

Bismuth telluride is used for energy conversion in thermoelectric generators. The functioning and efficiency of the generator is determined by its figure of merit, $\alpha^2/k\rho$, where $\alpha$ is the Seebeck coefficient, $k$ the thermal conductivity and $\rho$ the electrical resistivity. All these properties are temperature dependent.

Being a semiconductor, bismuth telluride has an electrical resistivity of the order of $10^{-3}$ ohm-cm. Hence, its measurement at room temperature was carried out by the four contacts method on rod shaped samples. AC current was used in order to prevent temperature gradients along the rods due to the Peltier effect, and the resulting electromotive force which would cause an error in the voltage measurement. The temperature dependence of the resistivity was determined by current and voltage measurements, using two contacts, at temperatures up to 280°C.

Samples were in sintered (polycrystalline) form and gave typical resistivity values of 1.9 and 1.6 mohm-cm for n and p type bismuth telluride, respectively. Anisotropies of about 17% for n-type samples, and of 13% for p-type samples were observed in the resistivity values in the three main directions. There was an increase in these values of about 60% for n type and 100% for p type samples when heated from room temperature to 280°C.

CONSTRUCTION OF A SYSTEM FOR MEASURING HEAT TRANSFER COEFFICIENTS
A. Melzer, M. Vaxman, and I. Shai

An experimental system simulating the thermal behavior of a fuel element channel in a nuclear reactor was put together. The system consists of a circulating pump, heat exchanger, and test section. The flowing water can be
pressurized up to a few atmospheres by means of a pressure tank with nitrogen as cover gas (see Fig. 8). Heating is achieved by a low voltage-high current dc power supply capable of producing 225 kW at 15 V.

![Schematic drawing of test rig](image)

**Fig. 8**
Schematic drawing of test rig

Heat transfer coefficients at forced convection and boiling up to the burn-out point can be obtained at different surface configurations and various flow and thermal conditions.

COLD WELDING UNDER VACUUM
G. Odis, G. Kimmel and J. Katz

A process for cold welding of metal plates was developed. A special device (Fig. 9) was used to achieve bonding with a vacuum between the metal plates.

The process consists of cold pressing around the periphery of the plates using the special device, followed by evacuation of the air from between the plates. The opening through which the air is evacuated is then sealed.
A method was also developed for examination of the bond quality. In pure aluminium and in copper very effective bonding strength was achieved. The bonding zone is shown in Fig. 10.
Nuclear power cells use radioisotope fuel as a heat source. Some heart pacemakers use plutonium-238 oxide fuel as the heat source. The fuel is contained in two small welded containers, one inside the other. The inner container is made of a tantalum − 10% tungsten alloy; the outer container is of Hastelloy C-276. A technique for welding the inner container, which contains the $^{238}$Pu oxide fuel, was developed. This included:

a) design, manufacture and operation of a glovebox for welding small containers containing plutonium.

b) design of jigs and fixtures to permit welding under optimal conditions (Fig. 11).

c) adaptation of tantalum welding procedures to welding the tantalum − 10% tungsten alloy.

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Fig. 11

Welding apparatus, including jigs and small container of Ta − 10% W, inside the glovebox

a) welding torch
b) small Ta − 10% W container, inside the chuck
c) chucks
d) positioning turntable (to drive the container during the welding)
The welded containers undergo visual quality control under a stereoscopic microscope, a leak detection test using a helium leak detector and metallographic examination. The metallography is done on representative samples taken from the production series of the welded containers. The final welding procedure for Ta - 10% W (Fig. 12) was developed in intermediate stages using stainless steel and tantalum containers as study specimens.

Fig. 12
A welded container of Ta - 10% W, and a container and lid before welding

REFERENCE:

DEVELOPMENT OF AN ELECTROMAGNETIC FORMING DEVICE
E. Falkenstein

Basic research concerned with establishing the equation of state of a solid metallic material requires the study of its mechanical and metallurgical behavior and characteristics under high strain, produced by high pressures over short time intervals. Electromagnetic forming, (EMF) is a method which seems to be particularly adaptable to obtaining this type of data. By this method a bank of energy storing capacitors is discharged through a spark gap switch and a coil connected in series. The high current passing through the coil induces an intense electromagnetic field which, in turn, induces strong eddy currents in the sample. The interaction of these eddy currents with the induced
electromagnetic field generates attractive or repulsive forces between the coil and the sample. These forces can be used to induce high strain rates.

The experimental set-up is shown in Fig. 13. The pressure developed in the coil during the discharge is expressed by (1):

\[ P = 0.1 \times 10^{-7} H^2 \]

where \( P \) is the pressure (psi) and \( H \) is the magnetic intensity (A turn/cm).

Fig. 13
Overall view of the electromagnetic forming device. The high voltage dc power supply is shown on the left; on the right the energy storing capacitor bank, above it the spark gap switch and the coil.

Pictures of samples deformed by this method are given in Fig. 14. A direct measurement of the pressure in the coil was not yet performed. The duration of the pressure pulse within the coil during the discharge is expressed by (2):

\[ t = K \left( \frac{c d A}{L} \right)^{1/2} \]

where,
- \( t \) - time (sec)
- \( K \) - const. of the device
- \( A \) - thickness of the flux pattern between the coil and the sample (mm)
The time of discharge, oscillation, and damping was measured. It is logical to assume that the effective pressure causing the deformation derives from the first three oscillating waves. The frequency of the oscillations lies in the kHz range.

Fig. 14
Samples deformed by EMF
a) copper cylinder, 26 mm O.D., 1 mm wall thickness
b) aluminium cylinder, 25 mm O.D., 0.3 mm wall thickness
The ratio between the relative heights of the consecutive peaks is measured on the vertical axis. An additional effect, noticeable during the discharge, was the build-up of high temperatures which caused local melting of the sample - the "skin effect", (Fig. 15).

Fig. 15
The skin effect as seen on a brass foil 0.15 mm thick

In order to make efficient use of the device, we tried to develop a coil best fitted to our purposes, taking into account the influence of its diameter, material, number of turns, and stiffness. We also tried to develop magnetic field shapers of various designs, based on tentative evaluations of the optimum ratio of O.D. to I.D., the total length, and the ratio of shaper length to coil length, geometry, etc. Some of the coils and field shapers are shown in Fig. 16.

Fig. 16
Coil and magnetic field shapers of various configurations and designs
We believe this technology to be of reasonable promise for short-time-high-pressure pulses, ensuring high rate changes.

REFERENCES:

AN AUTOMATIC MACHINE FOR CUTTING CAPILLARY TUBES WITH LASER BEAMS
Ch. Bachinsky, A. Kedem and G. Revesz

Attempts to manufacture small gas filled capillary tubes by standard manual glass blowing techniques were found to be impractical. A machine was therefore designed for automatic production of sealed capillary tubes, of lengths varying between 4 and 100 mm, especially very short pieces (4-6.5 mm). The minute sizes and the frail material required the development of non-standard methods for handling, feeding etc.

The machine works in the following sequence of steps:
1. mechanical transfer of raw material into the machine
2. continuous feeding of the tube to the cutting plane
3. simultaneous rotation of the sector being cut as well as the rest of the tube
4. a steady axial pull on the sector being cut, in order to avoid shrinkage during cutting
5. after cutting, release of pieces and their removal

A schematic drawing is given in Fig. 17. The magazine consists of an

---

Fig. 17
Schematic drawing of automatic cutting machine
1. base of the magazine, 2. wheel brake, 3. rotating support wheels, 4. cutting plane
inclinable plane, adjustable in width for various lengths of material. The tubes roll down the slope and are heaped near a wheel brake. A single tube is caught by the grooves on the perimeter of the wheel brake when the control system indicates that the cutting of the previous tube is completed.

The tube, transferred from the magazine, falls on pairs of rubber-covered rotating wheels, with its end positioned in the cutting plane. This end is caught by a chuck, which consists of three wheels rotating at the same speed as the supporting wheels. The chuck pulls the tube to the desired length. Then the tube is caught at its other end by upper holding wheels (not sketched); it is thus rotated and stretched at the same time. At this moment the laser beam shutter opens and closes and the newly cut piece is gravity-fed to storage.

**ELECTRIC DISCHARGE SLICING OF THERMOELECTRIC MATERIAL**

M. Lanxner

In spark machining, which is also called electric discharge machining, sparks are used to remove material, in a closely controlled manner, from an electrically conducting workpiece immersed in a dielectric liquid. This method of machining was used for accurately slicing specimens that are too delicate to withstand the forces involved in mechanical cutting. Samples of 0.6x0.6 mm in cross section and 10 mm in length were easily obtained using a wire slicer.

Two types of spark machines were tried: the Charmilles D-10 with a pulsed energy power supply and the Servomet SMD with a relaxation type generator. After the optimal spark energy and gap size were determined, both machines gave satisfactory results. Subsequently, a small electric discharge machine with an RC generator was designed and built in the laboratory, for especially delicate work.

A very brittle thermoelectric material such as Bi$_2$Te$_3$ was successfully sliced using the wire slicer. First, a moving wire was tried because it has the advantage of eliminating the tool wear factor, since new electrode material is presented to the work. On the other hand, frequent tool-to-workpiece shorts occurred across the spark gap. Then a fixed wire slicer was used, giving a more satisfactory and smooth cut. The main limitation on the use of fixed wires is in their tendency to break before the cut is completed. This was overcome by using a 0.25 mm dia. Ta wire strung between the arms of a plastic fork and tuned to a desired tension. With this device, cutting times were reproducible and continuous. When deep cuts of more than 25 mm were needed,
a cut of about 20 mm was first made; then, after advancing the worn segment of the wire, a second penetration completed the slicing.

Metal removal rate for the best operating conditions was 15-20 mm\(^3\)/min, and tool wear less than 1.5%.

A SEALED CONTROLLED-ENVIRONMENT CHAMBER FOR POLYMER GRAFTING WITH ELECTRON ACCELERATORS\(^1\)

A controlled-environment box for experimentation in the irradiation of flexible materials in sheet form (usually polymeric films) with electron accelerators (550 kV, 20 mA) was designed and built. The apparatus is suitable for use in studies of grafting to polymers in controlled environment. It permits grafting of liquid- or vapor-phase monomer onto a solid film both by pre- or post-irradiation techniques. The use of this chamber affords a favorable opportunity for the study of the optimum conditions for electron-accelerator use in possible industrial processes.

The apparatus essentially consists of an outer and inner section. The outer part is a shell of 0.7 cm thick 304 stainless steel (Fig. 18). The shell

![Fig. 18](image)

The outer shell of the controlled-environment chamber:
(a) titanium-foil window; (b) indium O-ring; (c) sealing flanges; (d) funnel; (e) needle valve; (f) Edward's Wilson seal
is fitted with a 25 μm thick titanium-alloy foil window (a) which is practically transparent to the penetration of electrons of 250 kV energy and above. A vacuum-tight connection between the foil and the shell is made by an indium O-ring (b), and sealing flanges (c). The shell is also equipped with a funnel (d), which is connected through a needle valve (e) to a tube connected by a vacuum-tight Edward's Wilson seal (f), which extends into the shell.

The inner part, the rolling system, is built on a frame which is inserted into the box (Fig. 19). It contains two cylinders (A), on which the treatable film is rolled (B). It is possible to roll the film in either direction.

Fig. 19

The rolling system:
(A) cylinders; (B) film for treatment;
(C) bevel gears; (D) shaft; (E) dc motor;
(F) Edward's Wilson seals; (G) solenoids;
(H) dipping bath; (I) vacuum gauge;
(J) thickness-indicating plate
Each of the cylinders can be separately attached by means of bevel gears (C) to a shaft (D) which is connected to a dc motor (E). The shaft enters the chamber through an Edward's Wilson seal (F). The shaft is connected into the required position (with regard to direction of rolling) by means of one of two solenoids (G), so that only one of the cylinders at a time is attached to the shaft via one of the gears. The film is rolled through a small bath (H) containing the liquid monometer which is not in the direct path of the electron-beam window. The rolling system is introduced into the outer shell and closed vacuum tight by screws and a 0.3 cm neoprene rubber gasket. The rolling system also has a pipe connection to a vacuum gauge (I) and pump through which the system is evacuated. An electro-mechanical device is provided to give a continuous indication of the thickness of the rolled film on one of the cylinders and to reverse the direction of rolling when the desired amount of film has been irradiated. This is accomplished by plate (J) pushing a shaft through another Edward's Wilson seal (F).

REFERENCE:

HIGH PRESSURE CELLS
J. Gross and E. Rapoport

For NQR experiments under hydrostatic pressure a large sample should be used. Therefore large volume pressure cells had to be designed and constructed. Two 4 cm - bore cells are currently being used in these experiments and can operate to 14,000 atm. A 5.6 cm - bore cell for 10,000 atm, and another, 1.27 cm - bore, designed for 36,000 atm for high pressure differential thermal analysis are under construction.

High pressure is generated by a 250 ton Kennedy-type hydraulic press. Since the highest grades of steel, even after most appropriate heat treatment, cannot withstand pressures above 8000 atm, the design had to be such as to avoid stresses beyond the elastic region of the material used. This was achieved by making the chamber of several supporting rings, so dimensioned that they serve mutually as peripheral pressure chambers one for the other; see Fig. 20.
Fig. 20
Schematic diagram of the high pressure chamber
1) set of three pressed rings to achieve pre-compression in the chamber bore
2) upper piston
3) pressure chamber
4) lower seal

Each cell is constructed from three or four supporting rings, one pressed into the other. The calculated difference between the outer diameter and respective bore of the next ring is on the order of 0.01 cm. As a result, the rings are in a state of precompression, which may be described as being in the negative range of the elasticity curve, but still in the elastic region. The optimal sizes were obtained by an IBM-370 computer program and after special heat treatment the rings were ground to a high finish to the respective sizes. Strain hardening does not occur since the stretching which follows a pre-compression does not reach the yield point of the material.

For magnetic and electrical measurements, special seals were designed, in order to introduce leads into the chamber.

A PRESS FOR HIGH LOADS
J. Gross and E. Rapoport

A Kennedy-type double press, double frame apparatus was constructed with a 250 ton lower hydraulic ram and a 125 ton upper hydraulic ram. The hydraulic power unit and control were also constructed. In normal routine operation the upper press provides end load on the high pressure cell assembly and the lower ram generates the high pressure. For certain applications the two rams can be combined in series to give a total of 330 tons.
The cell assembly is placed between the plates of the upper and lower frames. The stroke of each ram is 190 mm (this is also the stroke of each frame).

Pressure may be raised gradually and the rate of pressure increase can be controlled. Pressure can be maintained over a long period of time.

A diagram of the press is given in Fig. 21.

Fig. 21
Diagram of the high load press
1. upper frame  2. upper piston
3. lower frame  4. spacers
5. pressure chamber  6. lower piston

DISPERSION CELL FOR LASERS
Z. Miller, J. Daniel, M. Katz, G. Revesz and S. Zveigenboim

A device was designed for initiating reactions via a CO₂ pulsed laser on various materials under vacuum. This set-up was used for preliminary laser-plasma studies before the Nd:glass laser was operational.

The requirements for the design were as follows:
(a) vacuum of 10⁻⁵ Torr.
(b) provision of a number of openings for inserting measuring instruments, and for observing the process taking place.
(c) provision of a lens-holder for focusing the laser beam on a target in the center of the cell.
(d) provision for the targets (rods of different materials up to 5 mm diam) to be rotated during the experiment in a helical motion, for thorough scanning of the material.
The reaction cell (see Fig. 22) is made from a stainless steel tube, 142 mm O.D. and 200 mm long. On the circumference of the cylinder there are 7 openings, 6 of which are covered with glass discs of 1" diam, and sealed with O-rings and lock nuts. One opening opposite the lens holder is provided with a germanium diaphragm of 1" diam.

Fig. 22
Dispersion cell for lasers
1. dc motor 2. main lead screw
3. rotary feed through
4. target holder 5. target
6. lens-holder 7. cylindrical body

The helical motion of the target is obtained by a mechanical system consisting of a dc motor with controlled speed up to 40 RPM, rotating a screw through an Edward's rotary shaft. The screw is provided with a chuck for rotation of various diameters. The device is remote controlled.
A DEVICE FOR CHANGING X-RAY FILM UNDER VACUUM
A. Kedem and D. Salzmann

A device was developed for feeding X-ray film to be exposed to X-ray radiation emitted from laser-produced plasmas, (see page 94). The film is placed behind absorbers of various thickness and cut-off energies. From the relative blackening of the film one can derive the intrinsic temperature in the plasma. The problem of having to break the vacuum in the chamber to change the film after every exposure was overcome by this device. The system was designed for convenient change of film for approximately 20 daily experiments.

A simple compact mechanism was built (Fig. 23) to withdraw and return film into the magazine. A closed chain loop drives a catch along two coordinates.

Fig. 23
Mechanism for automatic positioning of X-ray plates
1. driving arm 2. y-axis bar 3. catch 4. frame
5. X-ray plates 6. diamond thread of bar (2)
7. coupling

The catch pulls one frame at a time out of the magazine, returning it after exposure. Then the catch moves to the adjacent film and repeats the operation. Both the feeding mechanism and the magazine for 10 film holders (20 exposures) are located in a light- and vacuum-tight chamber, which is connected to the target-chamber through a 4" VAT valve. The magazine automatically opens when introduced into the chamber and closes when taken out for transfer to the dark room.
A REMOTE-CONTROLLED X-Y-Z POSITIONER FOR LASER BEAM TARGETS
A. Tuval, M. Katz, G. Revesz and R. Herman

A device was designed and built to centrally position minute spherical pellet-targets to be hit by a laser beam in laser induced fusion experiments (see page 85). The pellets are held on fine wires in the target chamber, Fig. 24. Positioning is accomplished by means of a central rod (45 cm in length), which has four independent motions, controlled by 4 stepping motors, mounted outside the target chamber. Transfer of motion is made possible by means of a large bellows connection to the vacuum chamber.

Fig. 24
Schematic drawing of target positioner
1. bellows 2. wall of target chamber
3. catch 4. rotating base with 5 levers
5. target holding lever

During operation the transfer rod is rotated about its axis, and with every 72° of rotation a new target holder is brought to the central position. The mechanism consists of a minute lever, which touches a stationary catch and turns on its fulcrum until the wire enters the path of the incident beam.
A MOTOR DRIVEN MECHANISM FOR THE ELECTRON MICROSCOPE CAMERA

II. Admon, M. Marelli, I. Verskin and B. Yusuv

A motor driven mechanism was built for the camera of the JEOL JEM-7A electron microscope. The device consists of a geared two-directional motor, three limiting microswitches, a transmission, and a control system. The microswitches are mounted on discs, which are pre-adjusted accurately to stop the motor when the frame holder, with two photographic plates in it, reaches one of three positions: loading, ready for first plate exposure, ready for second plate exposure. The system is operated by a single push button knob, and is protected against misoperation.

The system requires minor alterations in the electron microscope itself, and is adjustable to other models of JEOL electron microscopes, such as JEM-7, T7, T8, 120, 150, 200A, 200B.

A DUAL-PURPOSE X-RAY SET-UP FOR VIEWING AND RADIOGRAPHY

D. Kedem, Z. Miller and M. Katz

X-ray set-ups are mainly used either for radiography or for viewing on a fluorescent screen. In our case, there was a need for an instrument capable of serving both purposes.

An apparatus was built in order to allow the X-ray machine to revolve 180° from viewing to radiography, (Fig. 25). It is remote controlled.

Fig. 25
Set-up for rotating the X-ray machine
a) X-ray machine
b) roll bearing
c) stand
d) driving chain
e) 180° motor
In order to protect the operator from radiation, a protective cell was built—a metal frame with walls made of wood sandwiched with lead. The cell is provided with a fluorescent screen covered with a lead glass, while in the back there is a door which can be opened by a cable connected to a motor (Fig. 26).

Fig. 26
Schematic diagram of the X-ray radiography apparatus
1. rope-drum motor 2. frame 3. tension pulley 4. cable 5. door 6. door-track

A TRANSPARENT FURNACE FOR TEMPERATURES UP TO 1000°C
S. Tuval, M. Katz and G. Revesz

A special furnace was designed to permit continuous visual inspection of crystal growing processes, up to 1000°C.
The furnace itself (Fig. 27) consists of a quartz tube, around which the heating coil is turned. The outer wall is made of three 10" diam Pyrex tubes spaced by 2 lava rings to compensate for thermal stresses. The inner surface of the tubes is half-coated with gold, reflecting the infra-red, but not interfering with visual surveillance.

Fig. 27
Schematic drawing of the furnace
1. outer Pyrex tube 2. quartz tube
3. lava heating coil holders
4. 1500 W Kanthal heating coil
5. lava spacers

Additional lava rings were designed to support the heating coil, in order to maintain the distance between it and the outer Pyrex tube.

DEVICE FOR MEASURING GAS EXCHANGES BETWEEN BODIES OF WATER AND THE ATMOSPHERE*

A device was designed for measuring radon concentration in sea water or lakes, as well as gas exchange between water and the atmosphere.

In an existing experimental set-up for preliminary measurements, a noble gas bubbles through the water sample and active particles are collected on

*This work was performed for the Weizmann Institute, Rehovot
special filters (Gellmann, Polipore, etc). The particles activate a scintillator and with the aid of a photomultiplier, the accumulated activity is determined. Since the replacement and handling of the delicate filters is usually difficult, and the decay time of the trapped material causes time delay, the main problem was to design an easy and simple method for filter exchange and cleaning, and a set-up for continuous measurements.

Instead of developing special seals and means for filter exchange, the problem was solved by using a commutable mount for the detector unit. Alternate positioning of the detector unit (scintillator and photomultiplier) between two separate filtering stations permits intermittent use of two counting stages, and the delay between successive measurements can be decreased.

The device itself, schematically shown in Fig. 28, consists of 2 independent counting cells (1), separated by plastic valves. They can be connected

![Fig. 28](image-url)

Schematic drawing of the measuring device
1. counting cell 2. filter-holding screen
3. photomultiplier 4. scintillator
5. rotatable cover plate 6. closure disc for the second cell
alternately to the outer vessel, which contains the sample under investigation. The filters are supported by a stainless steel screen (2) and sealed by O-rings tightened by an easily demountable frame. The filter is changed by placing the new filter on the screen, adding the O-ring and fastening the frame to the bottom of the cell. The scintillator (4) is set 1/8 in. from the filters and adjacent to the photomultiplier (3).

The detector unit (3,4) is bayonet mounted on the cover plate (5). A half-turn of the cover plate around its fulcrum transfers the detection unit to the second cell. A closure-disc (6) prevents penetration of light and the outer atmosphere during the turn of the cover plate; in the usual measuring position an O-ring seals off the gap between the cover plate and the cells.

The main housing is made of PVC. Aluminium parts are black anodized and PTFE impregnated. Parts which are not directly exposed to a possibly corrosive atmosphere are made of blackened brass.
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