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MOTOROLA INC SCOTTSDALE ARIZ GOVERNMENT ELECTRONICS DIV

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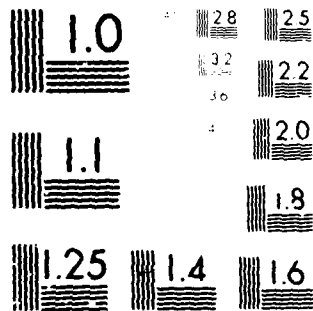
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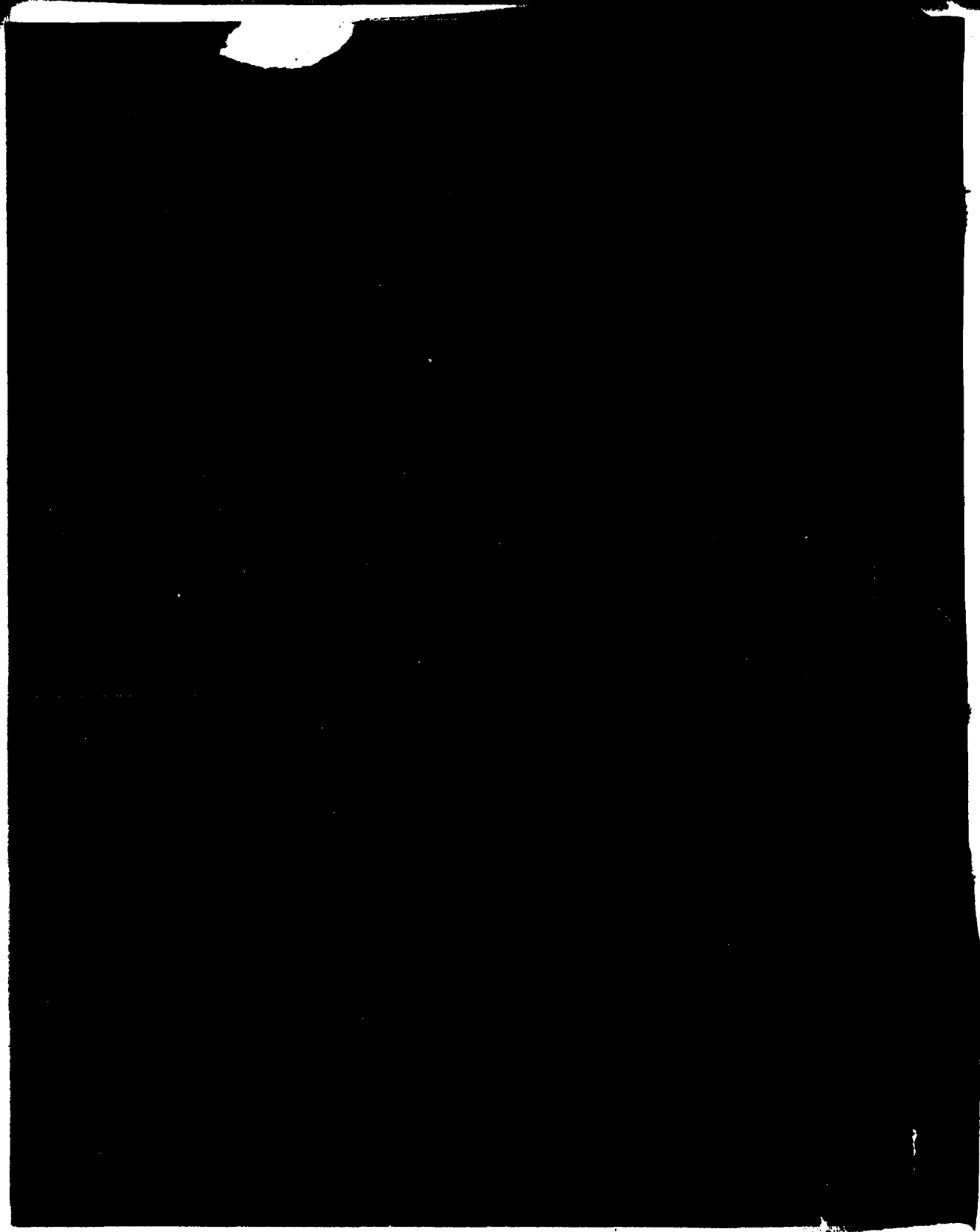
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The program consists of two major task areas comprising an interactive numerical/experimental approach. Task I involves the numerical computation of the key SAW properties for doubly rotated quartz substrates for the purpose of locating promising angular ranges with properties superior to the singly rotated cuts now in existence. More detailed calculations follow to refine the angular coordinates in order to specify cuts for experimental verification in Task II. In Task II, sets of substrates with promising orientations identified in Task I will be prepared and SAW device patterns will be fabricated for evaluation of the key SAW properties. The experimental results of this task will be correlated with the theoretical predictions and an iterative process develops for refinement of both theoretical and experimental parameters. As the program proceeds, working SAW device models will be delivered as a demonstration of progress and an indication of the future potential of the doubly rotated cuts. Depending upon the progress made and time and budget limitations, additional properties in the area of nonlinear elasticity will be investigated. This report contains the result of Task I and part of Task II.

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SECTION 1

INTRODUCTION

1. PROGRAM OBJECTIVE

The objective of this program is the exploratory development of doubly rotated cuts of quartz possessing superior Surface Acoustic Wave (SAW) properties for applications involving environmentally hardened devices. The key properties examined and optimized both theoretically and experimentally are: first, second and third order Temperature Coefficients of Delay (TCD), piezoelectric coupling factor, power flow angle, Bulk Acoustic Wave (BAW) inverse velocity surfaces, leaky waves, and sensitivities of the above quantities to misorientations and manufacturing tolerances.

2. PROGRAM SCOPE

The program consists of two major task areas comprising an interactive numerical/experimental approach. Task I involves the numerical computation of the key SAW properties for doubly rotated quartz substrates for the purpose of locating promising angular ranges with properties superior to the singly rotated cuts now in existence. More detailed calculations follow to refine the angular coordinates in order to specify cuts for experimental verification in Task II. In Task II, sets of substrates with promising orientations identified in Task I are prepared and SAW device patterns fabricated for evaluation of the key SAW properties. The experimental results of this task are correlated with the theoretical predictions and an iterative process develops for refinement of both theoretical and experimental parameters. As the program proceeds, working SAW device models will be delivered as a demonstration of progress and an indication of the future potential of the doubly rotated cuts. Depending upon the progress made and time and budget limitations, additional properties in the area of nonlinear elasticity will be investigated.

3. TECHNICAL APPROACH SUMMARY

To accurately characterize the properties of doubly rotated quartz, three basic capabilities are essential:

- a. Theoretical approach and associated computer software which will accurately and quickly locate promising zero TCD cut angles and characterize the other key SAW parameters
- b. Source of rotated quartz substrates of superior quality which can be quickly fabricated and the angular orientation which can be determined with a high degree of precision
- c. Required fabrication facilities and measurement tools to accurately determine the key SAW device parameters.

In the theoretical area, this program has characterized two basic theoretical approaches for the identification of zero TCDs on rotated cuts of quartz. For this study, two computer programs available at Motorola are used. The first program calculates the first, second and third order TCDs of rotated cuts using a finite difference method. This technique is simple, well established, and has been used for analytically determining the temperature coefficient curves for singly and doubly rotated cuts of quartz. To more accurately refine the temperature coefficient properties, a second program which encompasses lattice skewing effects is used. This more complete theoretical approach is based on the work of Sinha and Tiersten¹; its utility has been verified.

The final theoretical work is the characterization of the other key parameters with standard SAW programs used routinely for material characterization and device development.

Accurately oriented quartz bars, supplied by Motorola, Carlisle, are cut, lapped and finely polished at Motorola. A mechanical polishing procedure is used. During this program, several substrates from a single bar with incremental angular deviations about a promising angular position are fabricated. By careful organization of the angle selection and cut procedures, a substantial savings in time and money is achieved.

The angular orientation of the doubly rotated substrates are defined to an accuracy of within ± 5 minutes using X-ray diffractometry. Equipment used includes Laue pattern X-ray equipment, X-ray diffractometers, and precision wafer cut and polishing equipment.

A complete SAW test area and optical laboratory form the basis for evaluating the key SAW parameters of the doubly rotated quartz delay lines, oscillators and resonators. The equipment will be set up for rapid display and recording of the SAW parameters.

¹"On The Temperature Dependence of the Velocity of Surface Waves in Quartz", B.K. Sinha and H.F. Tiersten, Proceedings of the 32nd Annual Symposium on Frequency Control, 1978, pp. 150 - 153.

SECTION II

TECHNICAL DISCUSSION

The following section discusses the technical approaches used in this program. A comparison of numerical approaches is made and the numerical approach used is described in paragraph 1 (Task I). Experimental techniques (Task II) will be outlined in paragraph 2.

1. INTRODUCTION

Quartz is the most commonly used substrate for fabricating Surface Acoustic Wave (SAW) devices. In SAW narrowband filter, oscillator, and resonator applications, the temperature stability of the device is an important design parameter. Currently, almost all SAW devices fabricated on quartz use the ST-Cut, which exhibits a parabolic frequency dependence in temperature. For many applications, the temperature dependence of devices fabricated on ST quartz is too large. Thus it is desirable to find crystal cuts with superior temperature performance. Of course, many other design parameters must be considered when choosing a crystal cut. Some of the more important ones are the piezoelectric coupling coefficient, acoustic losses, dependence of device performance on cut misorientation, excitation of bulk modes, and beam steering angle. These parameters are all easily determined for a given cut.

The objectives of this program are to find crystal cuts which exhibit zero temperature coefficients of delay so that there will be no frequency-temperature dependence observed in temperature stable oscillators, resonators and filters. We have used computer models to investigate the temperature dependence of different cuts of crystal for SAW devices.

Defining τ as the delay time for an acoustic wave to propagate between two points on the surface of the crystal, we wish to find orientations for which τ is constant in temperature, or more formally $(1/\tau)(d\tau/dT)|_{T=25 \text{ degrees C}} = 0$.

If F is the frequency of a SAW resonator, we have $(1/F)(dF/dT) = -(1/\tau)(d\tau/dT)$. Of course, we would also like the higher order derivatives to be as close to zero as possible, or $(1/2\tau)(d^2\tau/dT^2)|_{T=25 \text{ degrees C}} = 0$, etc.

Letting l be the length between two points, τ is simply given by $\tau = (l/V)$, $(1/\tau)(d\tau/dT) = (1/l)(dV/dT) - (1/V)(dV/dT)$.

We have computer programs for calculating τ as a function of the stress, the dielectric and piezoelectric constants of a substrate material. Furthermore, we have at our disposal the temperature variation of those constants for quartz allowing one to calculate $(1/V)(dV/dT)$ by a finite difference method (note that higher order terms can be calculated the same way). If the crystal expansion coefficients are known, it is then a simple matter to calculate $(1/\tau)(d\tau/dT)$ for any particular orientation. Perturbation

programs developed by Sinha and Tiersten to calculate $(1/\tau)(d\tau/dT)$ are also available. Combined with a search method, we are able to find cuts for which first order temperature coefficient of frequency vanishes.

a. Calculation of Temperature Coefficients

It has been shown that determining the temperature dependence of τ (time delay) is equivalent to determining the temperature dependence of F (frequency) via the relation $F \propto 1/\tau$.

Since our experimental data is derived from frequency measurements, we determine the frequency characteristics of the devices. The relation between the temperature coefficient of frequency (TCF) and temperature coefficient of delay (TCD) are related as follows (See Appendix E):

$$\alpha_F^{(1)} = -\alpha_\tau^{(1)} \quad (1)$$

$$\alpha_F^{(2)} = -\alpha_\tau^{(2)} + (\alpha_\tau^{(1)})^2 \quad (2)$$

$$\alpha_F^{(3)} = -\alpha_\tau^{(3)} + 2\alpha_\tau^{(1)} \alpha_\tau^{(2)} - (\alpha_\tau^{(1)})^3 \quad (3)$$

where $\alpha_F^{(i)}$ is the i th order TCF, $\alpha_\tau^{(i)}$ is the i th order TCD.

Using the relations above, one can always relate one set of the temperature coefficients to the other.

The various procedures outlined in the following sections will yield the quantities $\alpha_v^{(i)}$, $i = 1, 2, 3$, with $V(T) \cong V(T_0)(1 + \alpha_v^{(1)} dT + \alpha_v^{(2)} dT^2 + \alpha_v^{(3)} dT^3)$ and $dT = T - T_0$.

The problem of interest is not only, however, in finding the $\alpha_v^{(i)}$'s but in finding the delay time τ and the frequency dependence F of a device. The frequency dependence $F(T) = F(T_0)(1 + \alpha_F^{(1)} dT + \alpha_F^{(2)} dT^2 + \alpha_F^{(3)} dT^3)$ is a function of not only V , but of $\ell(T_0) = \ell(T_0)(1 + \alpha_\ell^{(1)} dT + \alpha_\ell^{(2)} dT^2 + \alpha_\ell^{(3)} dT^3)$, the spacing between reflectors in a resonator (or the length of the delay line in an oscillator)

From the above relations and $(1 + X)^{-1} \cong 1 - X + X^2 - X^3$ if $X \ll 1$, we see that:

$$F = V/\ell \cong \{ V (1 + \alpha_v^{(1)} dT + \alpha_v^{(2)} dT^2 + \alpha_v^{(3)} dT^3) \} / \ell_0 (1 + \alpha_\ell^{(1)} dT + \alpha_\ell^{(2)} dT^2 + \alpha_\ell^{(3)} dT^3) \quad (4)$$

$$\cong F(T_0) \{ 1 + \alpha_v^{(1)} dT + \alpha_v^{(2)} dT^2 + \alpha_v^{(3)} dT^3 \quad (5)$$

$$- \alpha_\ell^{(1)} dT - \alpha_\ell^{(1)} \alpha_v^{(1)} dT^2 - \alpha_\ell^{(1)} \alpha_v^{(2)} dT^3$$

$$- \alpha_\ell^{(2)} dT^2 - \alpha_\ell^{(2)} \alpha_v^{(1)} dT^3 - \alpha_\ell^{(3)} dT^3$$

$$+ (\alpha_\ell^{(1)})^2 dT^2 + (\alpha_\ell^{(1)})^2 \alpha_v^{(1)} dT^3$$

$$+ 2\alpha_\ell^{(1)} \alpha_\ell^{(2)} dT^3 - (\alpha_\ell^{(1)} dT)^3 \} \quad (6)$$

or

$$\alpha_1^{(1)} = \alpha_1^{(1)} - \alpha_1^{(1)} \quad (7)$$

$$\alpha_1^{(2)} = \alpha_1^{(2)} - \alpha_1^{(1)} \alpha_1^{(1)} + (\alpha_1^{(1)})^2 - \alpha_1^{(2)} \quad (8)$$

$$\alpha_1^{(3)} = \alpha_1^{(3)} - \alpha_1^{(1)} \alpha_1^{(2)} + \alpha_1^{(1)} (\alpha_1^{(1)})^2 \quad (9)$$

$$-(\alpha_1^{(1)})^3 + 2\alpha_1^{(1)} \alpha_1^{(2)} - \alpha_1^{(1)} \alpha_1^{(2)} - \alpha_1^{(3)}$$

giving the frequency dependence directly. The calculation of the temperature coefficients of velocity, $\alpha_1^{(1)}$, is achieved by calculating the phase velocity with the Finite Difference Technique or other techniques discussed below for a variety of temperatures. As the velocity is a function of temperature, a linear regression program is used in the finite difference technique to curve fit the data to a third order polynomial. The constants $\alpha_1^{(1)}$, $\alpha_1^{(2)}$ and $\alpha_1^{(3)}$ are thus obtained by optimum curve fitting of the data points to the polynomial. The temperature coefficients of length, $\alpha_1^{(1)}$, are found in standard references. It should be noted that the α_1 's also depend on the direction of propagation, and must be calculated for each direction of propagation considered by a simple geometrical transformation analogous to that used to rotate all of the other physical constants.

b. Rayleigh Wave

We will briefly discuss the Rayleigh wave solutions in their general form in this section. The coordinate system is defined with the Z or 1 axis being the direction of propagation and the -Y or 3 axis normal to the crystal surface. V_R will denote the Rayleigh wave velocity, $\beta_R = \omega/V_R$, the wave number, u_i (i = 1, 2, 3), the particle displacements along the 1, 2, or 3 axis, $u_4 = \phi$, the electric potential. Also, T_{ij} denotes the stress tensor.

$S_{ij} = (1/2)(du_i/dx_j + du_j/dx_i)$, the strain tensor, c_{ijkl} , the elastic tensor, ρ the density of the substrate, D, the electric displacement, E, the electric field, ϵ_{ij} the dielectric constant, e_{ijk} the piezoelectric constant. We also use Δ for the difference, where, for example,

$\Delta\rho = \rho(T) - \rho(T_0) = \rho(T_0)(\alpha_\rho^{(1)}dT + \alpha_\rho^{(2)}dT^2 + \alpha_\rho^{(3)}dT^3)$, and let P = power/unit width in the x direction.

We assume relations such as

$$T = -e \cdot E + c^E : S \text{ or } S = e^E \cdot E + S^E : T \quad (10)$$

$$D = \epsilon^S \cdot E + e : S \quad D = \epsilon^T \cdot E + d : T$$

$$\rho \partial^2 u_j / \partial t^2 - c_{ijkl} \partial^2 u_k / \partial x_j \partial x_l - e_{kij} \partial^2 \phi / \partial x_i \partial x_k = 0 \quad (11)$$

$$e_{ikl} \partial^2 u_k / \partial x_i \partial x_l - \epsilon_{ik} \partial^2 \phi / \partial x_i \partial x_k = 0$$

The general solution for a wave traveling on the surface can be written

$$u_j = \left[\sum_m C_m \alpha_j^{(m)} \exp(-(i\omega/V_j) \sum_{i=1}^3 b_i^{(m)} x_i) \right] \exp(i\omega t) \text{ for } j = 1 \text{ to } 4 \quad (12)$$

$$\text{For the Rayleigh wave, this reduces to } U_1 = \sum_{m=1}^4 C_m \alpha_j^{(m)} \exp(-i\beta_R b^{(m)} y) \exp(i\beta_R z - i\omega t) \quad (13)$$

where the coefficient c_m , $\alpha_j^{(m)}$ (weighting factors), β_R (wave number), and $b^{(m)}$ (complex decay constants) are to be calculated by the standard iterative procedure on a computer.

The fields are calculated as $E = \nabla u_4$ with $E_x = 0$, $E_y = (-i\beta_R b^{(m)})u_4$ and $E_z = (i\beta_R)u_4$.

c. Methods for Calculating the Temperature Dependence of the Rayleigh Velocity

In the following sections, four methods for calculating the temperature characteristics of the Rayleigh wave are discussed.

(1) Finite Difference Technique of Calculating Temperature Dependence of the Rayleigh Velocity

Before $TCD^{(1)} = (1/\tau)(d\tau/dT)$ can be calculated, one must first calculate the dependence of the Rayleigh wave velocity on temperature. The most straightforward method for doing this is the finite difference method. The Rayleigh wave velocities are calculated for different temperatures, yielding the values $V_i(T_i)$, $i = 1, 2, \dots, n$. This is done by first calculating the fundamental constants at the temperature T_1 of interest. The fundamental constants are then rotated into the coordinate system of interest. An iterative procedure is used to calculate a velocity V_i for which Christoffel's equation and the boundary conditions are satisfied simultaneously (see Appendix D). Simple finite difference techniques can be used to calculate $(1/V_i)(dV_i/dT)$, $(1/2V_i)(d^2V_i/dT^2)$, etc. For example, after calculating $V_i(T_i)$ for $T_1 = T_0$, $T_2 = T_0 + \Delta T$, $T_3 = T_0 - \Delta T$, we can use $(1/V_i)(dV_i/dT)$ at $T_0 \cong (1/V_0(T_0))(V_i(T_0 + \Delta T) - V_i(T_0 - \Delta T))/2\Delta$. Alternately, standard linear regression of polynomials may be employed to yield those coefficients. Another approach consists of calculating directly the frequency-temperature characteristics of the orientation for several widely differing temperatures. A measure of the temperature stability is then used. Letting $F(T)$ be the frequency of the device, the measure of deviation is calculated as

$$\begin{aligned} \text{RMS frequency deviation} &= \\ &= \left[\left(\sum_{i=1}^n (F(T_i) - F(T_0))^2 \right) / n \cdot F(T_0)^2 \right]^{1/2} \text{ with} \\ F(T) &= V_i(T) / \lambda_0 (1 + \alpha_L^{(1)}(\Delta T) + \alpha_L^{(2)}(\Delta T)^2 + \alpha_L^{(3)}(\Delta T)^3), \end{aligned} \quad (14)$$

although $\alpha_L^{(1)}$, $\alpha_L^{(2)}$, and $\alpha_L^{(3)}$ are calculated for purposes of comparison.

In much of the earlier work, the SAW velocities were calculated at three temperature points, $T_1 = -50^\circ\text{C}$, $T_2 = 25^\circ\text{C}$, and $T_3 = 100^\circ\text{C}$, to save on computer time. The following formulas were used for the calculations of first and second order temperature coefficients of velocity.

$$\begin{aligned}\alpha_V^{(1)} &= [V(T_1) - V(T_3)]/[V(T_2) (T_1 - T_3)] \\ &= [V(100) - V(-50)]/[V(25) \cdot 150]\end{aligned}\quad (15)$$

$$\begin{aligned}\alpha_V^{(2)} &= [V(T_1) + V(T_3) - 2 \cdot V(T_2)]/[V(T_2) \cdot 2 (T_3 - T_2)(T_2 - T_1)] \\ &= [V(100 + V(-50) - 2 \cdot V(25)]/[V(25) \cdot 2 (75)(75)]\end{aligned}\quad (16)$$

In the more recent works, six temperature points were calculated for each orientation to provide data for the linear regression analysis. The six temperature points were 100°C , 85°C , 75°C , -25°C , -10°C , and -50°C . The results were used to calculate $\text{TCF}^{(1)}$, $\text{TCF}^{(2)}$ and $\text{TCF}^{(3)}$.

(2) Perturbation Technique of Calculating Temperature Dependence of the Rayleigh Velocity

Perturbation theory may be applied to the problem of calculating the first, second and third order dependence of the Rayleigh velocity V , of a piezoelectric substrate, once the solution to the Rayleigh wave propagation at a temperature reference T_0 is known.

Perturbation techniques allow calculations of small changes in the solutions to a problem caused by small changes in the physical parameters of the problem, once the solution to the unperturbed problem is known. One can apply perturbation techniques either to boundary perturbation such as mass loading on the surface or to volume perturbations such as adding a thin conducting layer to the interior of piezoelectric substrates. As the boundary conditions are unaffected by changes in temperature while material constants such as c_{ij} are temperature dependent, one can apply the volume perturbation theory to the problem.

The general approach to the problem of determining the temperature dependence of V , will be as follows. First, the Rayleigh wave propagation problem will be solved in the standard way in its entirety at room temperature, T_0 . Given the solution of the problem at T_0 and the dependence of the physical constants (such as c_{ij}) on temperature at T_0 , one will apply the volume perturbation formula, calculating the temperature dependence of V . The dependence of V , on T is then used to calculate the frequency characteristics of the actual device given the thermal expansion coefficients as a function of temperature. At this point, the frequency temperature dependence of the substrate as a function of the crystal cut and direction can be thoroughly explored. See Appendix A for a complete discussion of this method.

(3) Approach of Sinha and Tiersten

The primary difficulty with the perturbation technique is that it does not take into account the change of coordinate systems induced by the thermal expansion in the material. This comes about because the material distorts as temperature changes. Thus, the set of axis is to which the fundamental elastic constants refer, which is fixed to the crystal, is no longer equivalent to the axis used to calculate V_s . This problem is elegantly solved by Sinha and Tiersten^{1,2}. The first simplification which occurs is that the density of the material remains constant with temperature. Furthermore, the $\alpha_i^{(0)}$ simply become $\alpha_i^{(1)} = \alpha_i^{(0)}$, as the length in this coordinate system does not change. The only difficulty is that the elastic constants previously used no longer refer to the proper coordinate system and must be rederived from the original experimental data. This procedure has already been carried out for the first order temperature derivation of quartz³ but has not been done for the second and third order coefficients. Nonetheless, the procedure yields more accurate results for the first order dependence. See Appendix B for a mathematical description of the salient features of this technique.

(4) Differentiation Method

A method for determining the theoretical temperature dependence of Rayleigh Surface Waves consists of formally differentiating the wave equation and boundary conditions. The boundary conditions and wave equation must be true at all temperatures, placing constraints on how the parameters of the wave equation may vary. In this technique, the derivatives of these equations with respect to temperature are set to zero and solved for the velocity-temperature dependence. This method follows the methods used by Bechmann, Ballato, and Lukaszek to compute the temperature dependence of the fundamental elastic constants from frequency data, except that the simplifying assumptions of assuming bulk wave solutions cannot be made. This method was later used by Hauden³ to search for temperature stable cuts of quartz. See Appendix C for a discussion of this method.

(5) Summary of Approaches

Of all the techniques presented, the finite difference technique satisfies all of the basic requirements for calculating temperature coefficients of delay. Arbitrary crystal structures may be

¹"On the Temperature Dependence of the Velocity of Surface Waves in Quartz," Sinha and Tiersten, 1978 Ultrasonics Symposium Proceedings, pp. 662-665.

²"Temperature Dependence of the Fundamental Elastic Constants of Quartz," Sinha and Tiersten, Proceedings of the 32nd Annual Symposium on Frequency Control, 1978, pp. 150-153.

³"Higher Order Temperature Coefficients of Quartz SAW Oscillators," D. Hauden, M. Michael, J. J. Gagnepain, Frequency Control Symposium (1978), pp. 77-86.

investigated once the density, piezoelectric, elastic, and dielectric constants and their temperature variation are known. When double precision on the computer is used and when the velocity over a large temperature range is calculated, it becomes a very accurate numerical approach. The computational efficiency of the finite difference method is not as high as some of the other techniques, owing to the need for repeated calculation of the surface wave velocity.

A comparison between the experimental results of Schulz¹ and Motorola's finite difference program adapted from Jones et al.² as shown in Figure 1. The results for this cut and many other orientations studied have been found to be very good. The slight shift of the analytical curve versus experimental curve can be explained by a crystal misorientation.

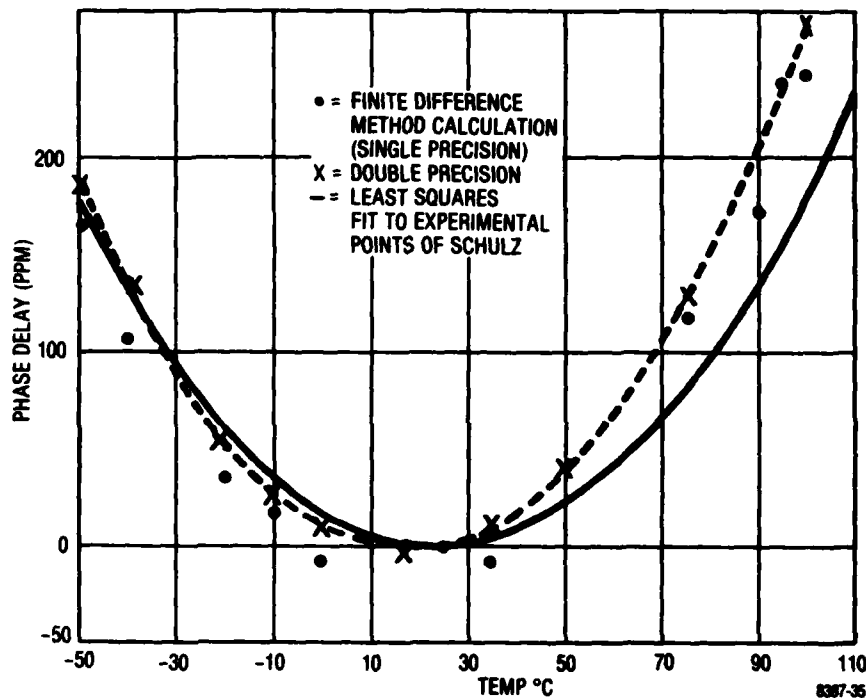


Figure 1. Finite Difference Method Versus Experiment ST-Cut (Quartz)

¹"Surface Acoustic Wave Delay Lines with Small Temperature Coefficient," Schulz, Manfred B., Proc. IEEE, Sept. 1970, pp. 1361-1362.

²"Numerical Computation of Acoustic Surface Waves in Layered Piezoelectric Media - Computer Program Descriptions", Jones, Smith, and Perry, Hughes Aircraft Company, Final Report, Air Force Cambridge Research Laboratories, Contract No. F19628-70-C-0027.

Figure 2 displays a phase delay versus temperature plot for the orientation (YXwlt) 56/40/27 in quartz obtained from Hauden's graphs². Using the differentiation approach, he calculated $\alpha_T^{(1)} = 0$, $\alpha_T^{(2)} = -0.04 \times 10^{-1} \text{ ppm}/^\circ\text{C}^2$, $\varphi_T^{(1)} = -22.7 \times 10^{-6} \text{ ppm}/^\circ\text{C}^1$ for a cut close to (YXwlt) 56/40/27. The Finite Difference approach was used to verify his first order calculation but is in disagreement on the second and third order calculations. This can be resolved by experiment.

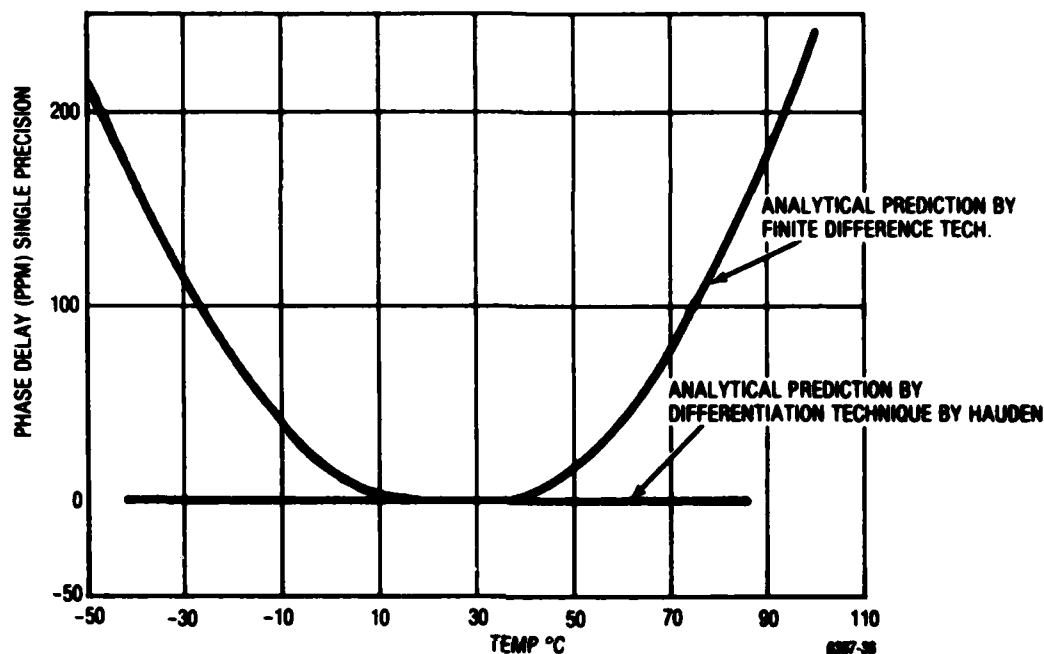


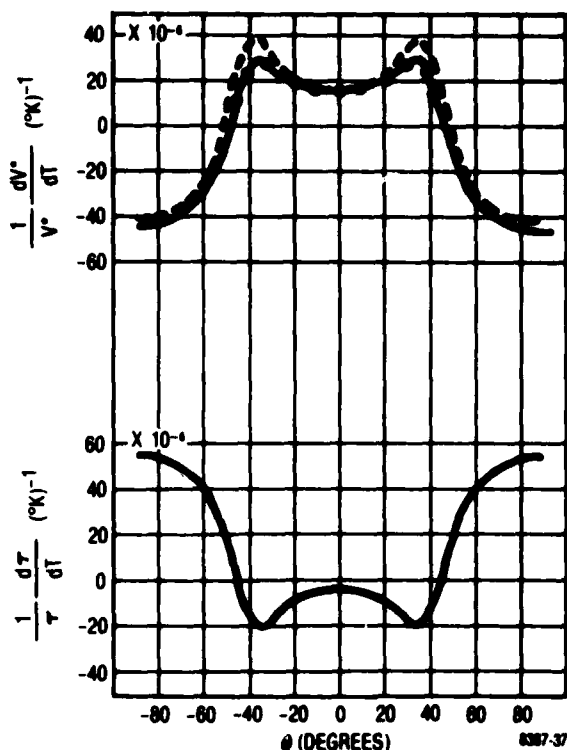
Figure 2. Finite Difference Method Calculation for Hauden's Cut (YXwlt) 56°/40°/27°

Tiersten's Perturbation program, while very difficult to extend to higher orders, is available for calculating the first order TCD.

Figure 3 shows the results of Tiersten's calculation¹ and compares those results with the Finite Difference method as well as experiment. The cut used for comparison is the AT-Cut. The improvement in accuracy is substantial. It offers the significant advantages of being quite cost efficient, as well as being more accurate in the first order on off-axis cuts, our primary area of interest. In the task of making quartz cuts along the surface of zero TCD, accurate values for the first order TCD prove more useful than the less exact values for the first, second, and third order TCD's provided by other methods, because it is a necessary (but not sufficient) condition for zero TCD cut to get a zero first order. Since it is the dominating term, it is important to first get an accurate first order zero TCD locus. Then one may search for the intersection of this locus with the zero second and third order terms with the finite difference technique.

¹"Temperature Dependence of the Fundamental Elastic Constants of Quartz," B. K. Sinha and H. F. Tiersten, Proceedings of the 32nd Annual Symposium on Frequency Control, 1978, pp. 150-153.

²"Higher Order Temperature Coefficients of Quartz SAW Oscillators," D. Hauden, M. Michael, J. J. Gagnepain, Frequency Control Symposium (1978), pp. 77-86.



TEMPERATURE COEFFICIENTS OF ACTUAL VELOCITY AND DELAY FOR SURFACE WAVES ON AT-CUT QUARTZ AS A FUNCTION OF PROPAGATION DIRECTION RELATIVE TO THE DIAGONAL AXIS AT 25°C. THE DOTTED CURVE SHOWS THE AVERAGE OF THE CALCULATED VALUES AT 0°C AND 50°C FROM REF. 1. THE CIRCLES ARE THE AVERAGE OF THE EXPERIMENTAL VALUES AT 0°C AND 50°C. GRAPH OBTAINED FROM REF 1

Figure 3. Tiersten's Method Versus Finite Difference and Experiment

(6) Investigative Approach

A necessary but not sufficient condition to find a temperature stable cut of quartz is that $\alpha_F^{(1)} = 0$. In practice, a sufficient condition for finding a zero temperature cut is that $\alpha_F^{(1)} = \alpha_F^{(2)} = \alpha_F^{(3)} = 0$. Thus every zero temperature cut must be on the locus of angles which satisfy the condition $\alpha_F^{(1)} = 0$. Thus the first problem is to locate accurately such cuts. Both the finite difference approach and Tiersten's method are being used now to calculate the TCF.

The approach used in this program is to identify the areas (angles) where $TCF^{(1)}$, $TCF^{(2)}$ and $TCF^{(3)}$ are relatively low by using the Finite Difference Approach and then define the exact orientation that has zero $TCF^{(1)}$ in those areas by the Sinha and Tiersten approach.

In case the condition $TCF^{(1)} = TCF^{(2)} = TCF^{(3)} = 0$ cannot be met, a compromise approach would be to find an orientation where the first and third order effects tend to cancel out in the temperature range of interest and to find the minimum second order effect orientation amount for those cuts. This approach would provide an effective low TCF cut of quartz for SAW application.

(7) Analytical Results on Zero TCF on Quartz

IRE standard angle definitions (YX wlt) PHI/THETA/PSI for quartz were used throughout the investigation¹. Consider the TCFs to be functions of these angles, which define an angular volume $0 \leq \text{PHI} \leq 30^\circ$, $-90^\circ \leq \text{THETA} \leq 90^\circ$, $0 \leq \text{PSI} \leq 180^\circ$, which spans the space of possible cuts and propagation directions. The set of points at which $\text{TCF}^{(1)}(\text{PHI}, \text{THETA}, \text{PSI}) = 0$ forms a surface in this angular volume. Likewise, the set of points at which $\text{TCF}^{(2)}(\text{PHI}, \text{THETA}, \text{PSI}) = 0$ also form surfaces in this angular volume.

Our object is to find a point where $\text{TCF}^{(1)} = \text{TCF}^{(2)} = \text{TCF}^{(3)} = 0$. If the surface of zero $\text{TCF}^{(1)}$ intersected with the surface of zero $\text{TCF}^{(2)}$, the result would be a line (or a point if the two surfaces are tangent to each other) of angular points on which $\text{TCF}^{(1)} = \text{TCF}^{(2)} = 0$. The intersection of this line with the surface on which $\text{TCF}^{(3)} = 0$ would yield a single point at which $\text{TCF}^{(1)} = \text{TCF}^{(2)} = \text{TCF}^{(3)} = 0$. Neglecting higher order terms, we would have found a temperature stable cut.

The calculated values of $\text{TCF}^{(1)}$ versus propagation angles are shown in Figure 4. The zero $\text{TCF}^{(1)}$ is identified by the areas where $\text{TCF}^{(1)}$ changes sign.

Using the Finite Difference approach with the available crystal constants, the calculated results show that the zero $\text{TCF}^{(1)}$ surfaces do not intersect with the zero $\text{TCF}^{(2)}$ surfaces, based on the interpolated results of the $10^\circ \times 10^\circ \times 10^\circ$ resolution. It is not likely that a finer resolution will provide contrary information because $\text{TCF}^{(1)}$ and $\text{TCF}^{(2)}$ are relatively slow varying functions as shown in Figure 4.

¹"Standards on Piezoelectric Crystals 1949," Proc. IRE 14, Dec. 1949, pp. 1378-1395.

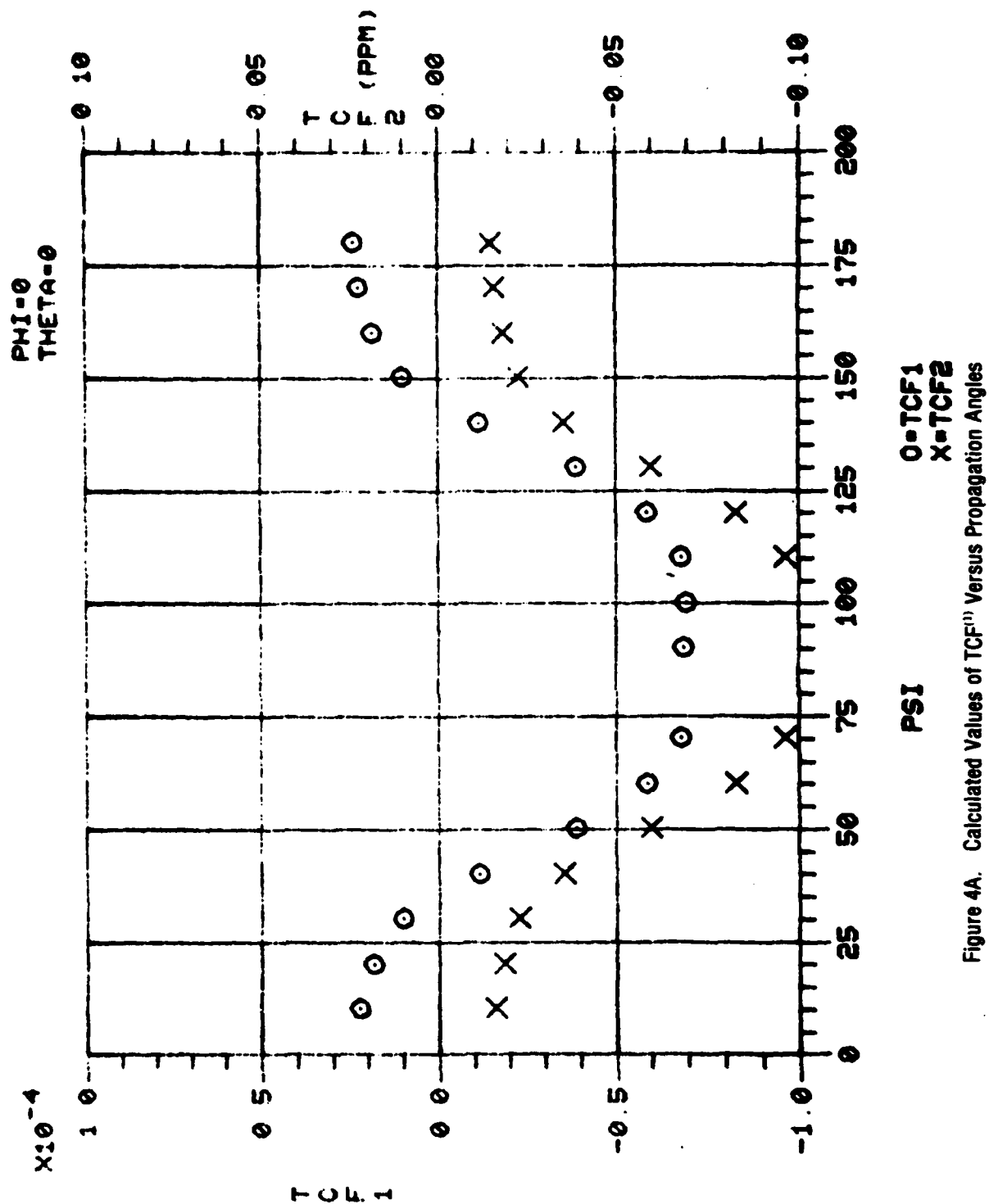


Figure 4A. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

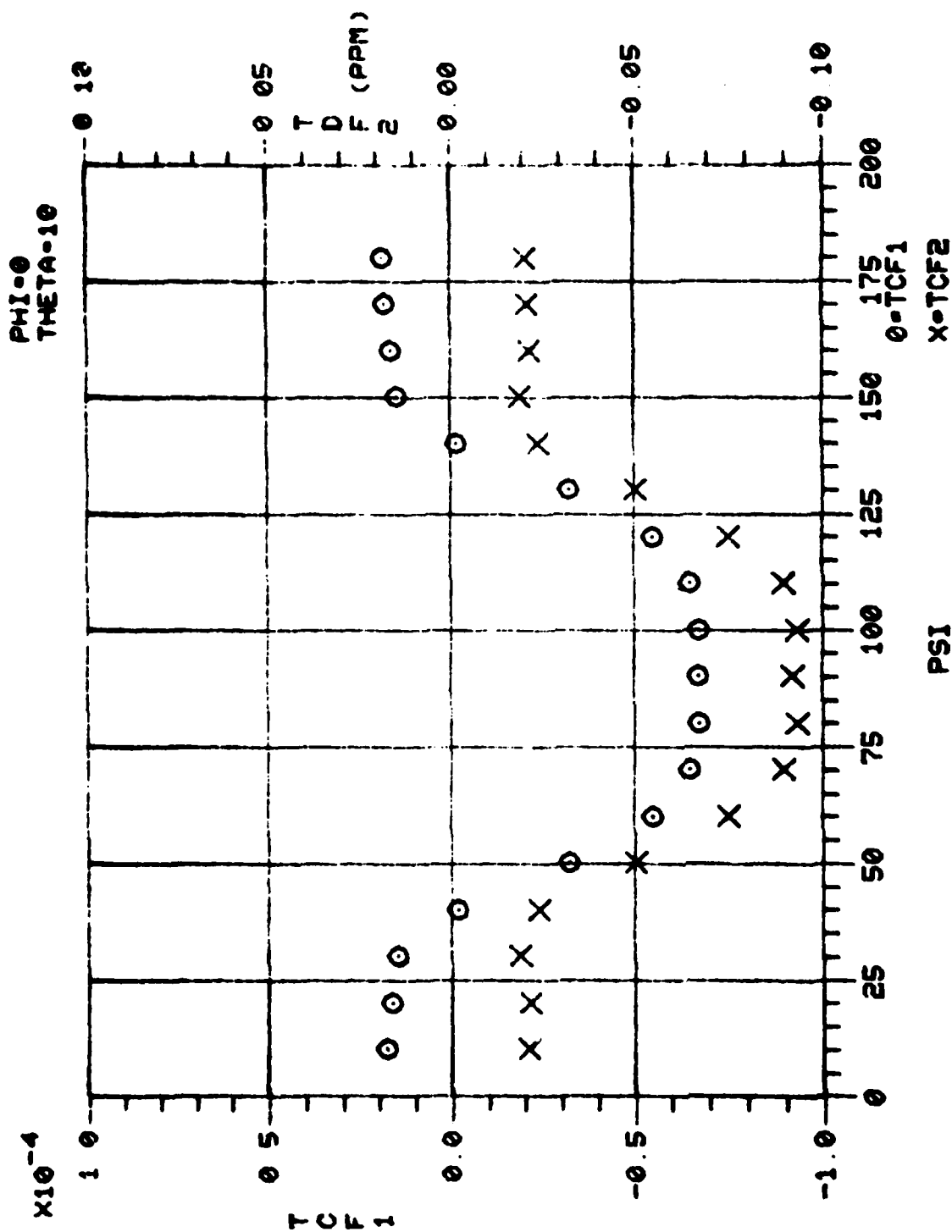
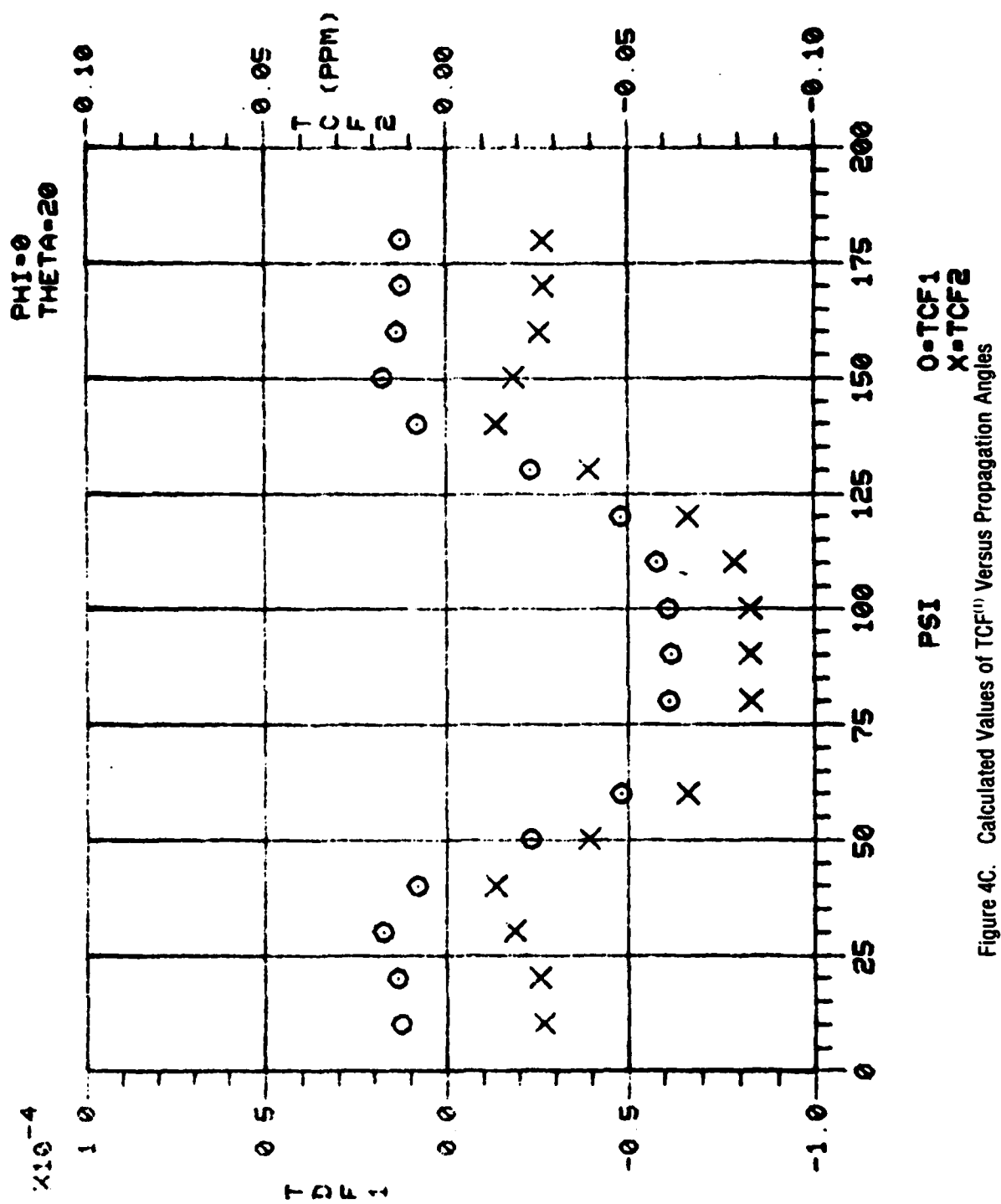


Figure 4B. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles



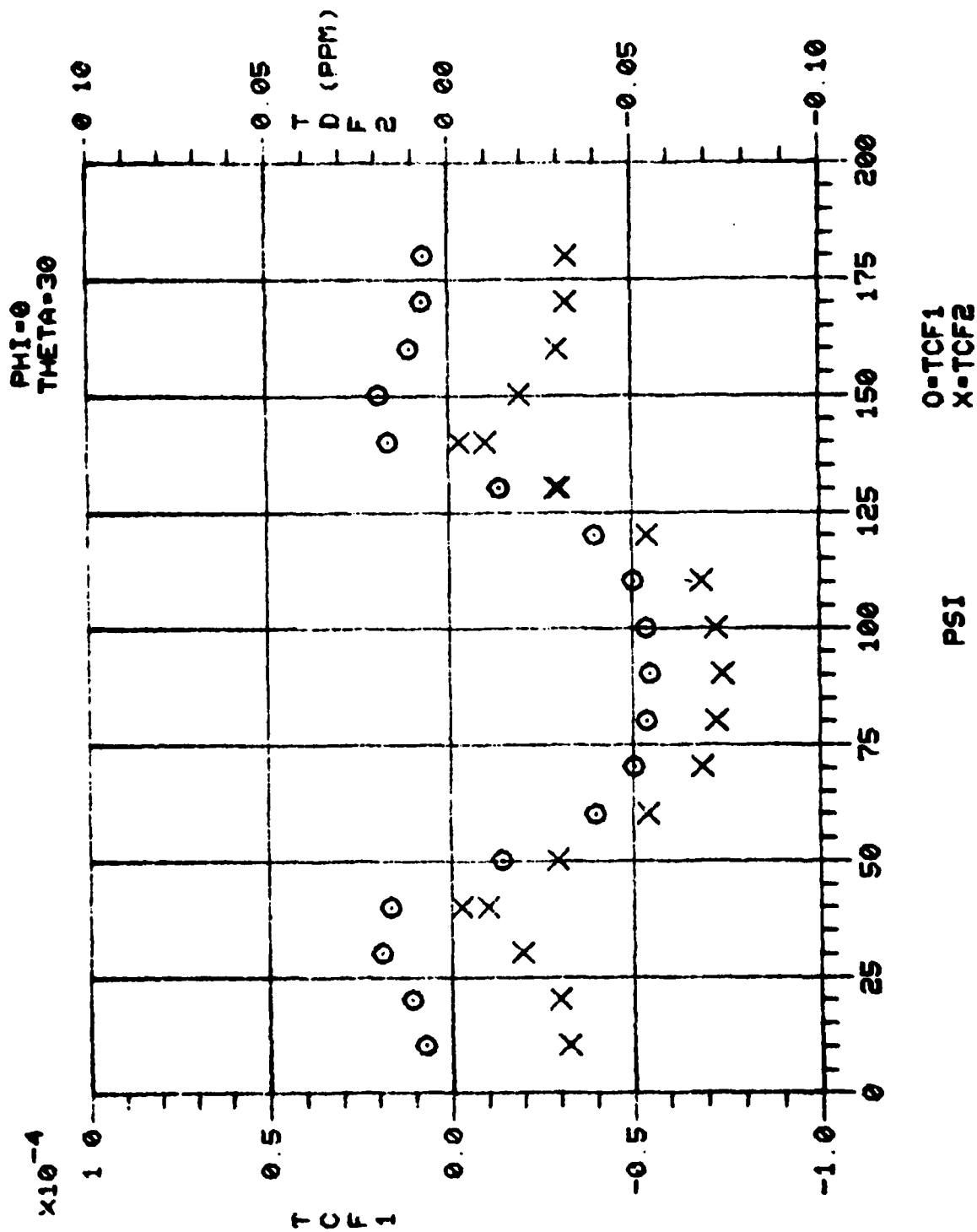


Figure 4D. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

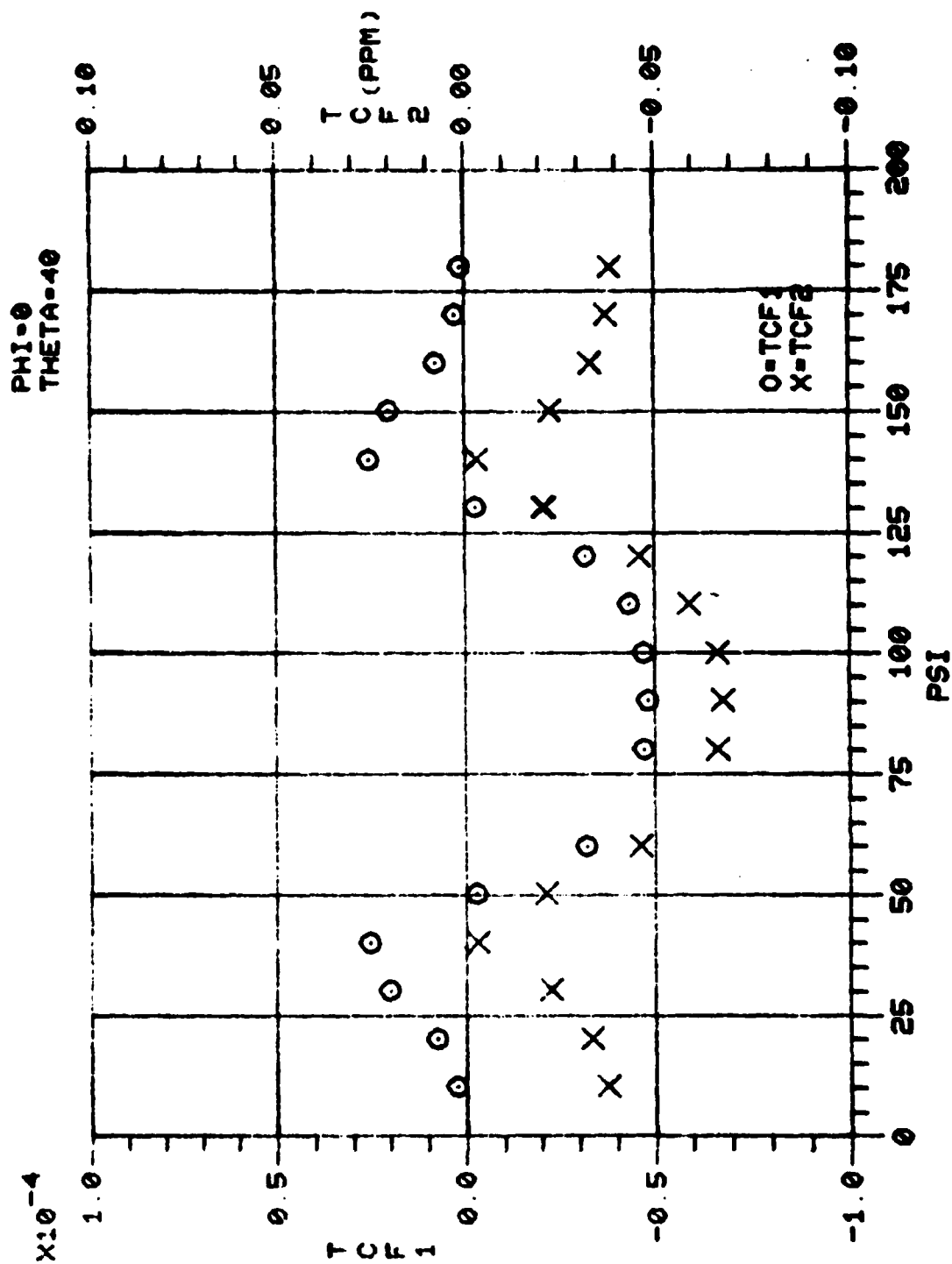


Figure 4E. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

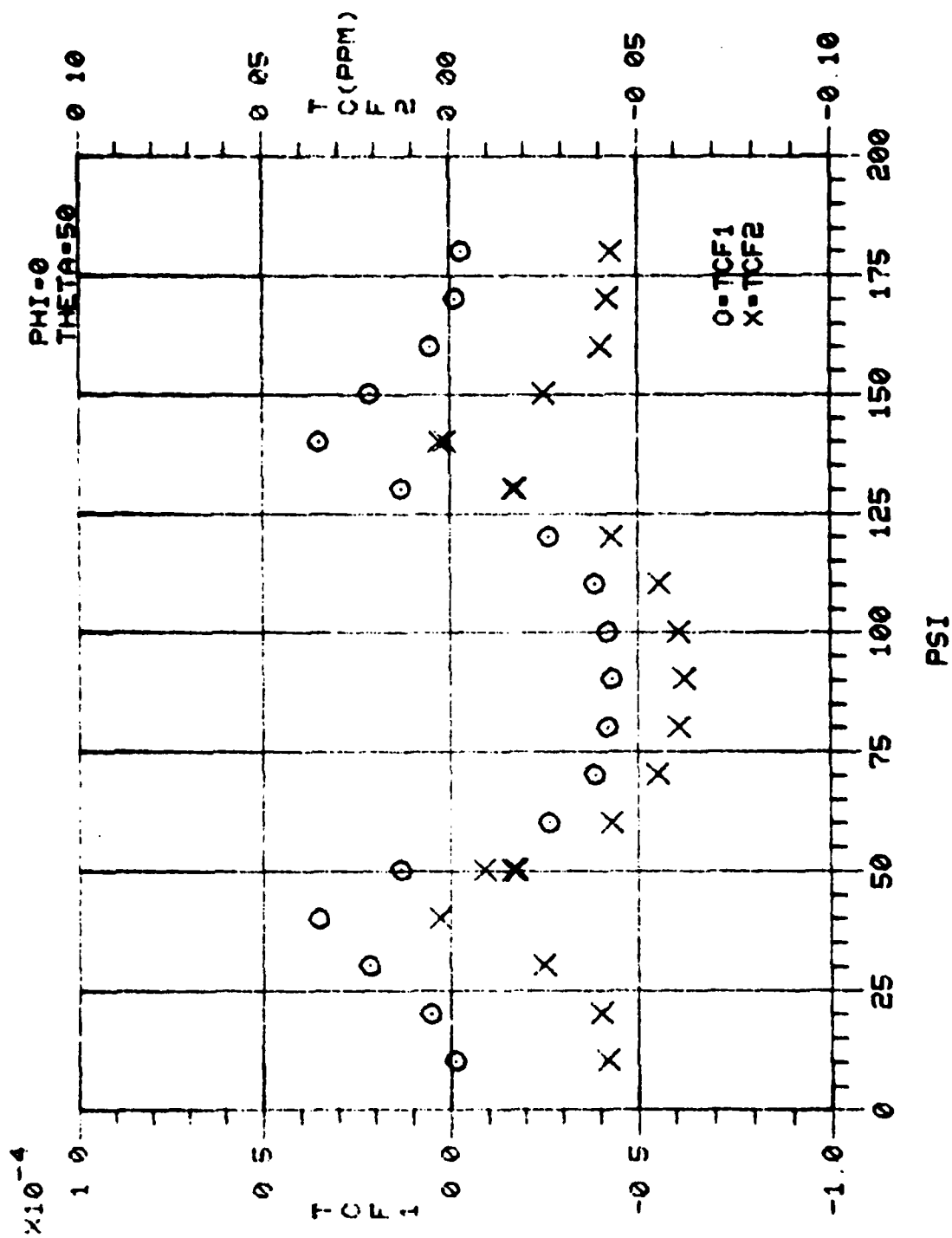


Figure 4F. Calculated Values of TCF(1) Versus Propagation Angles

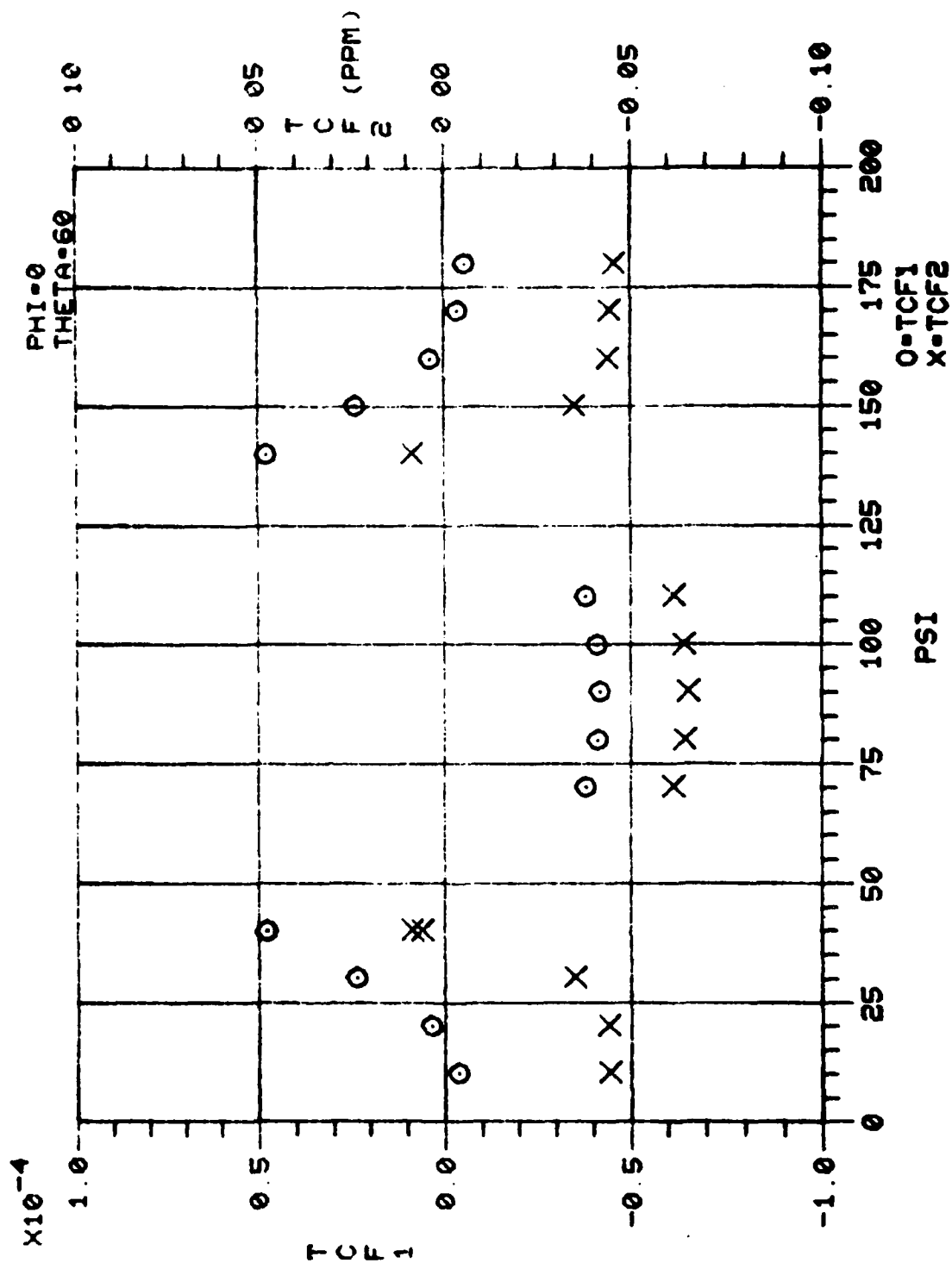


Figure 4G. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

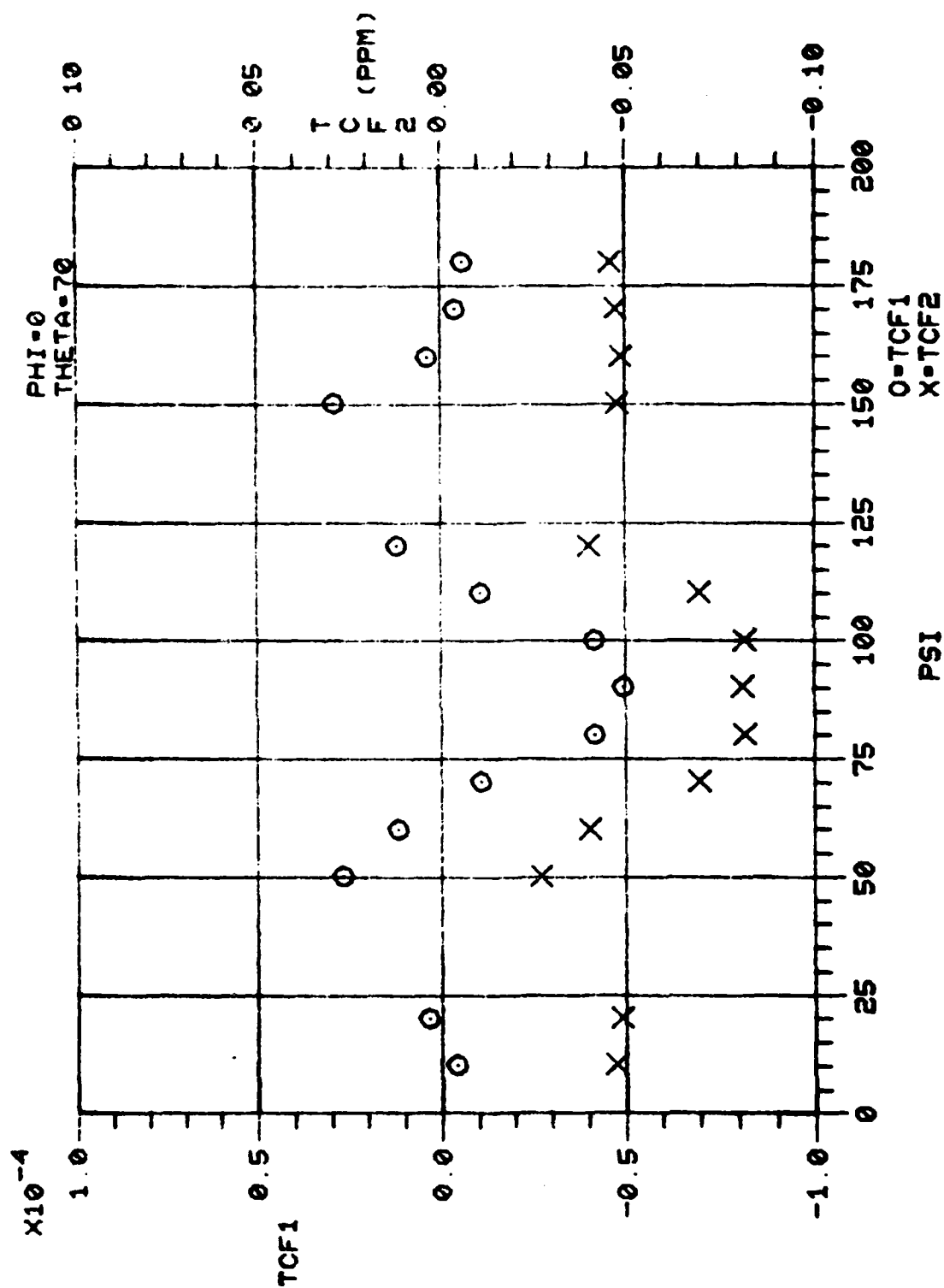


Figure 4H. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

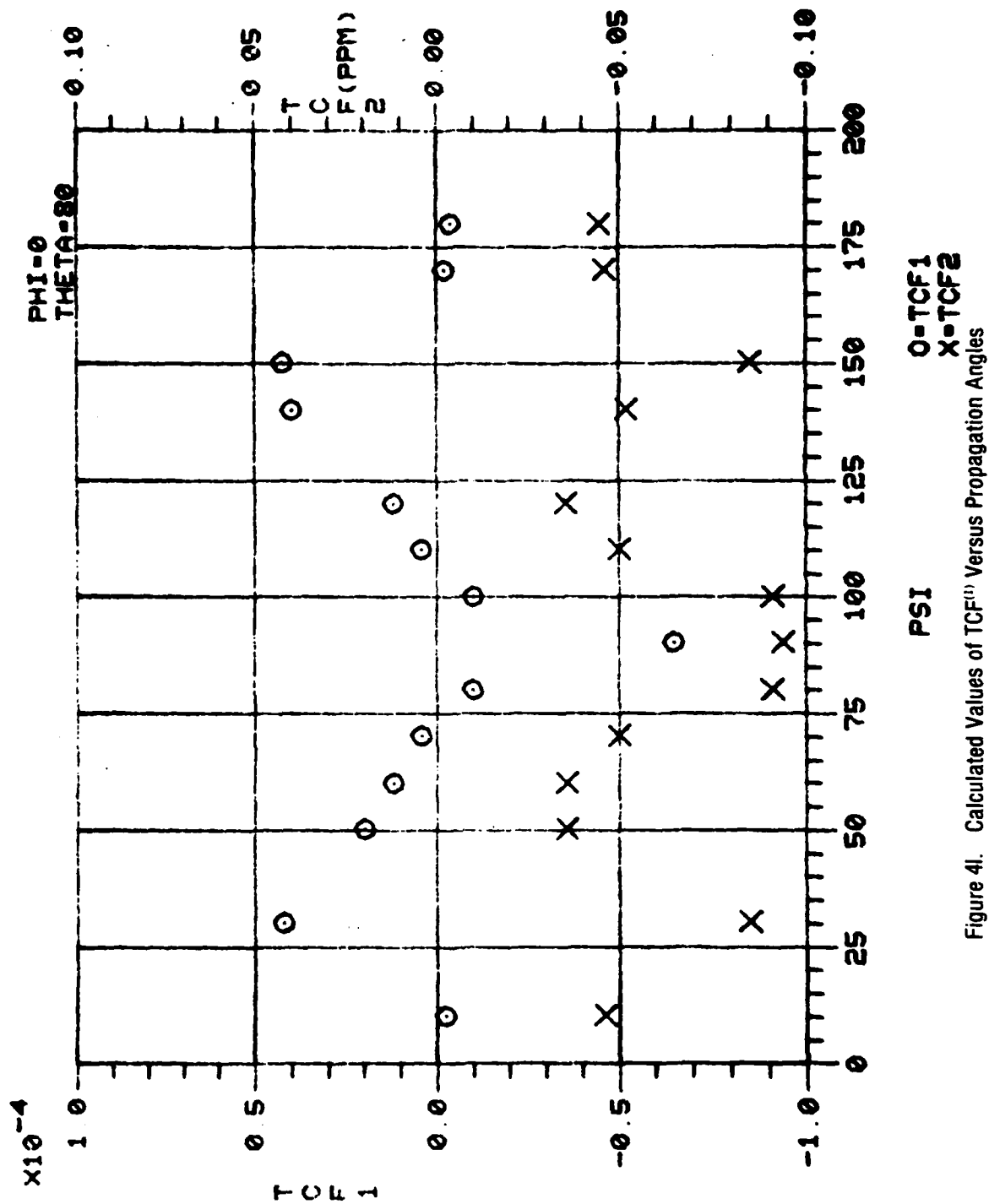


Figure 4I. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

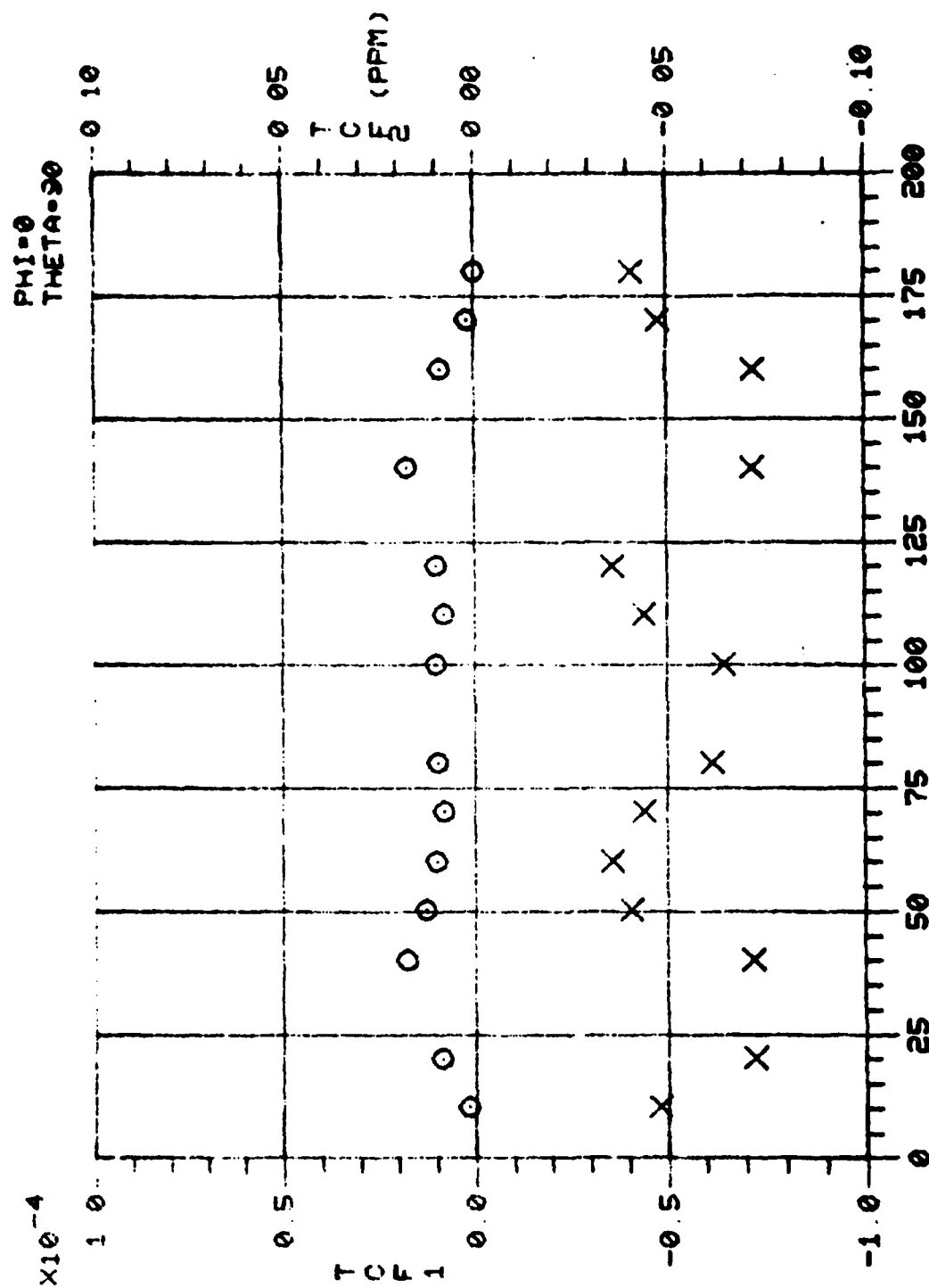


Figure 4J. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

O-TCF1
X-TCF2

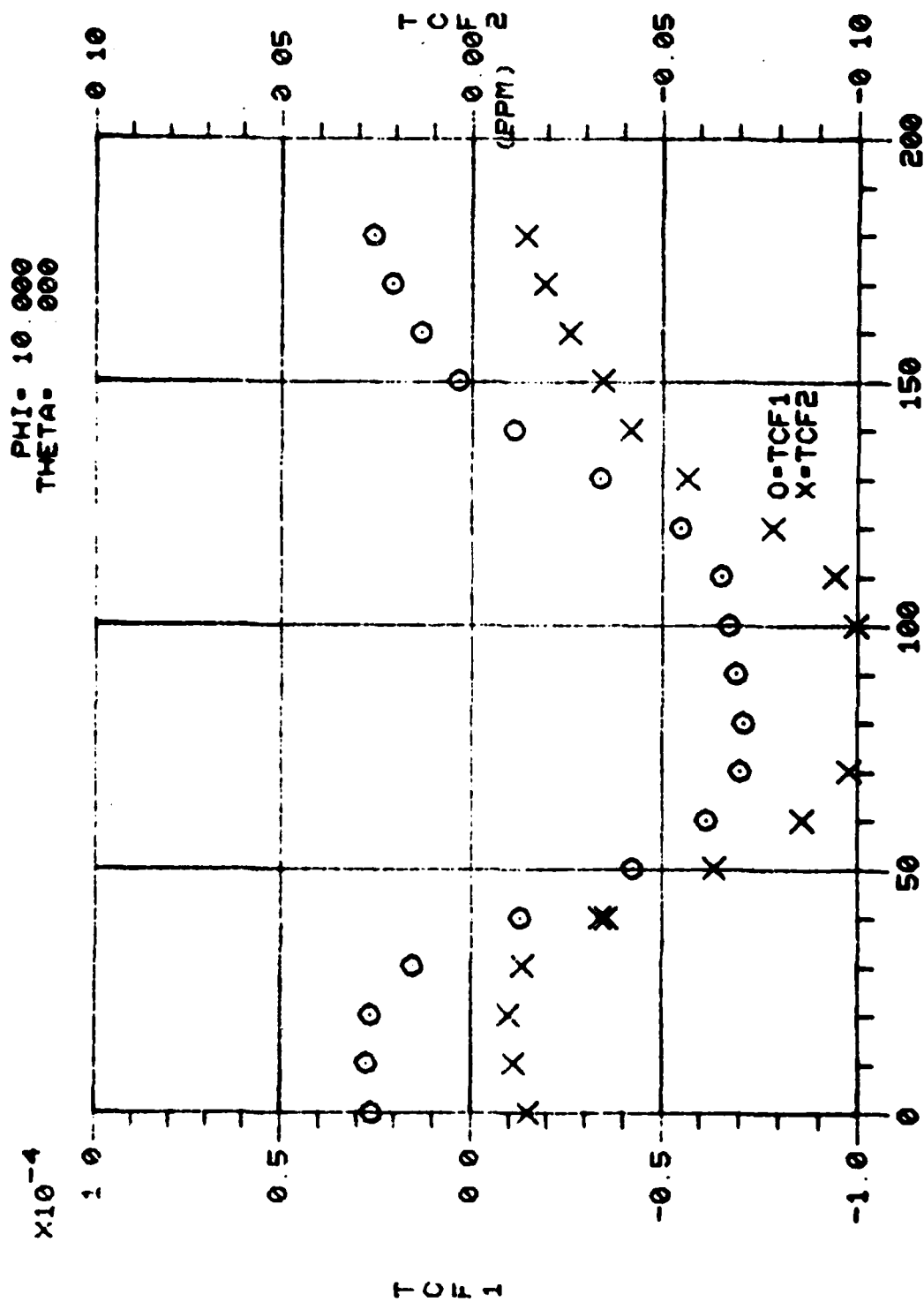


Figure 4K. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

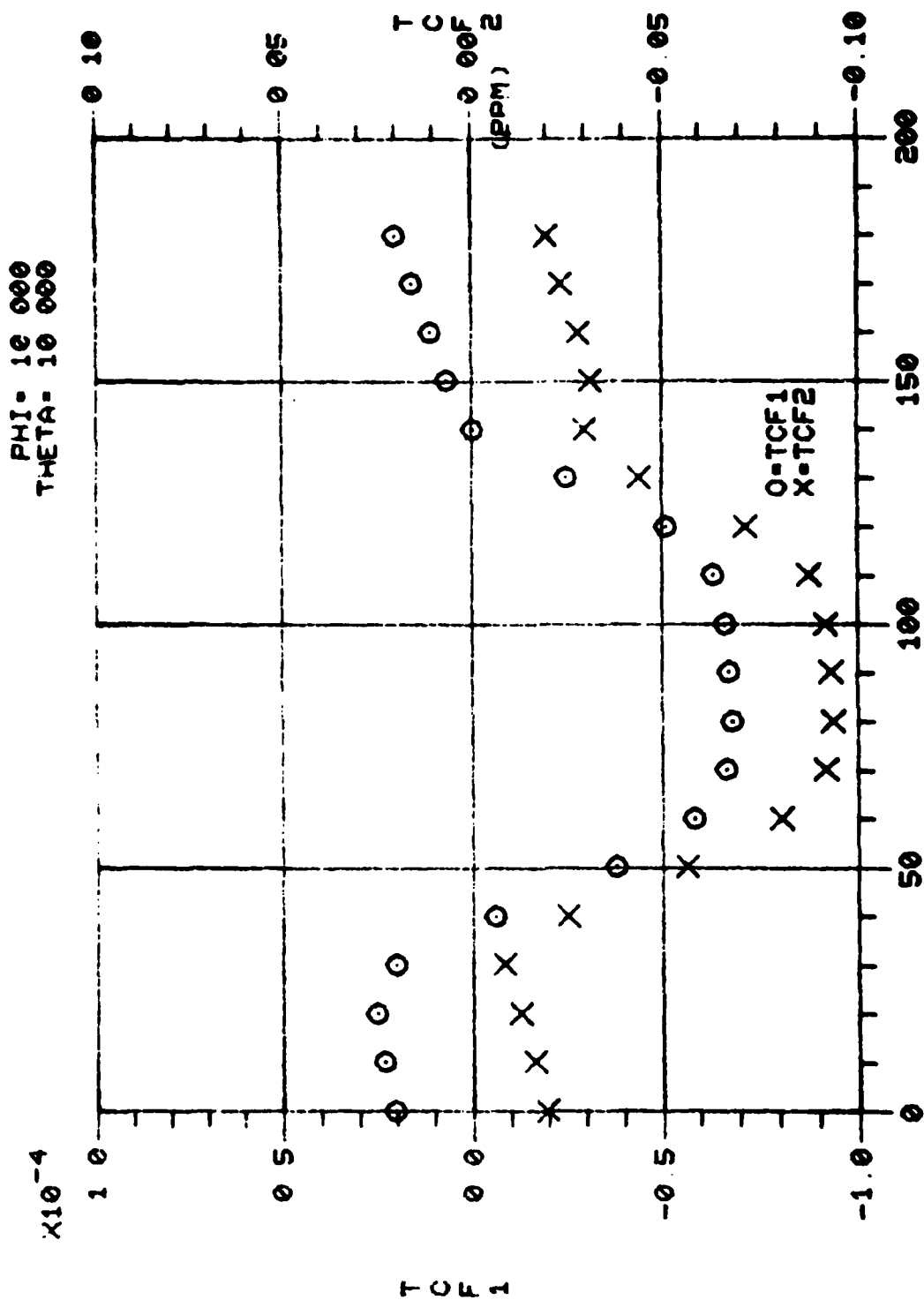
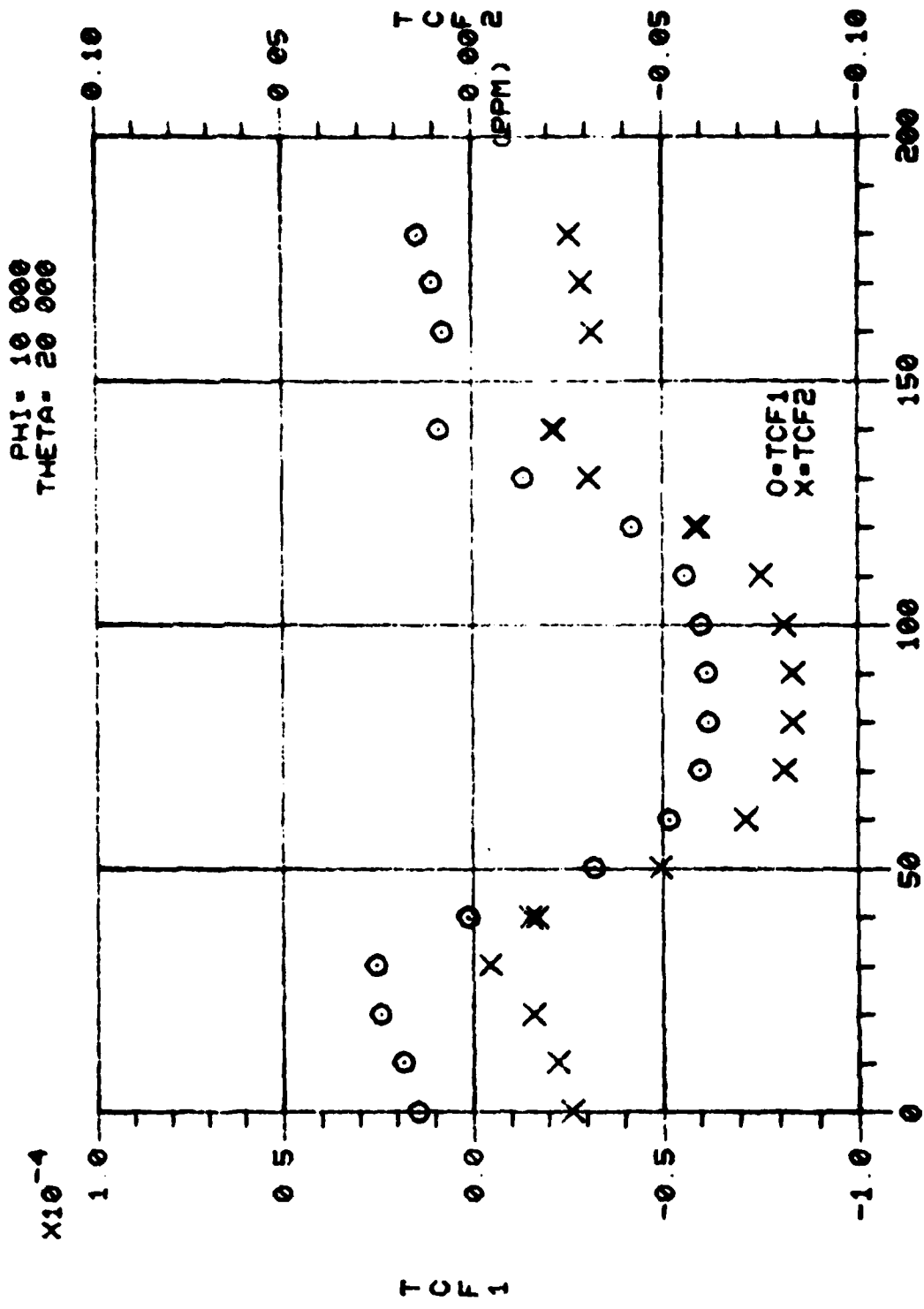


Figure 4L. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles



PSI
Figure 4M. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

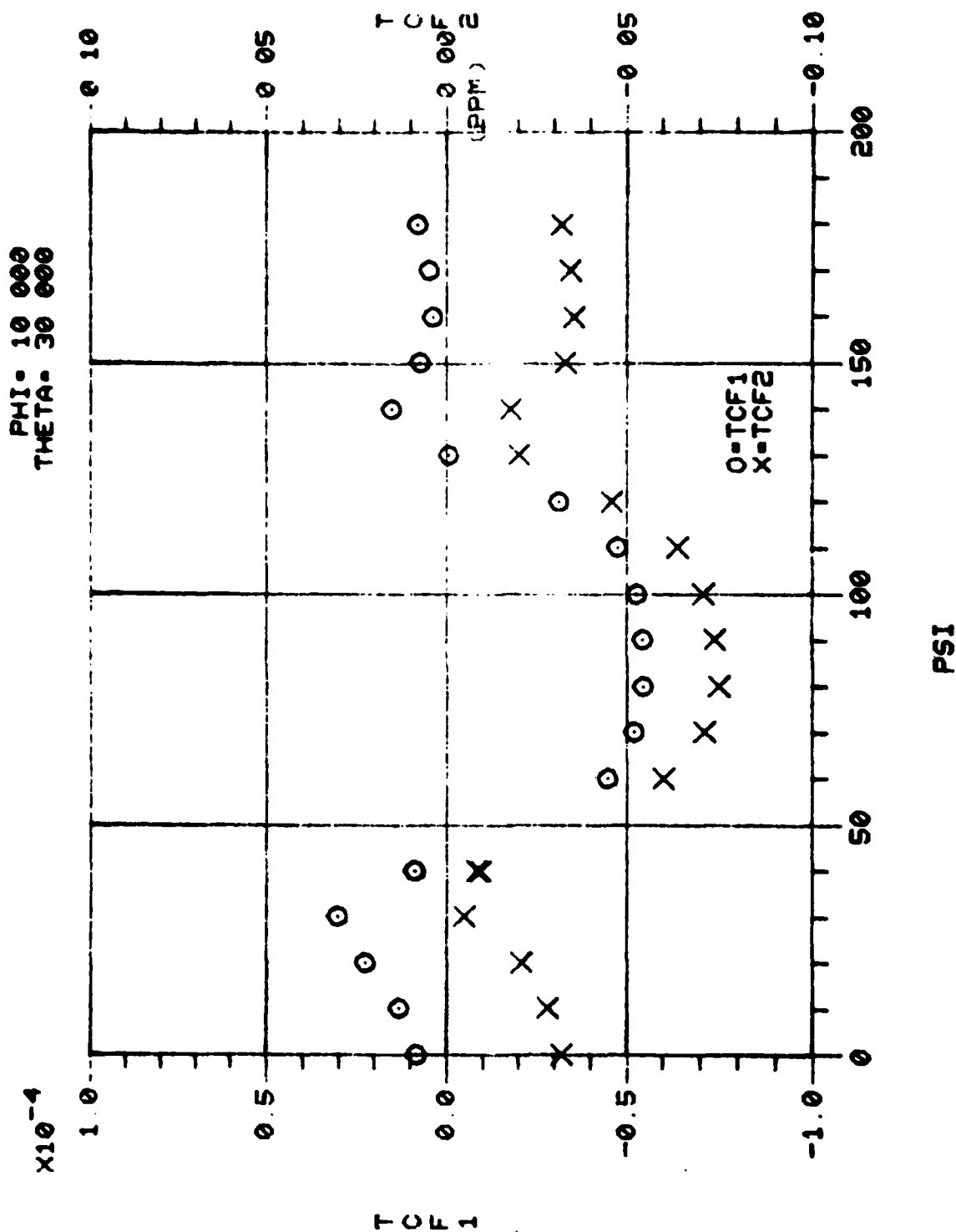


Figure 4N. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

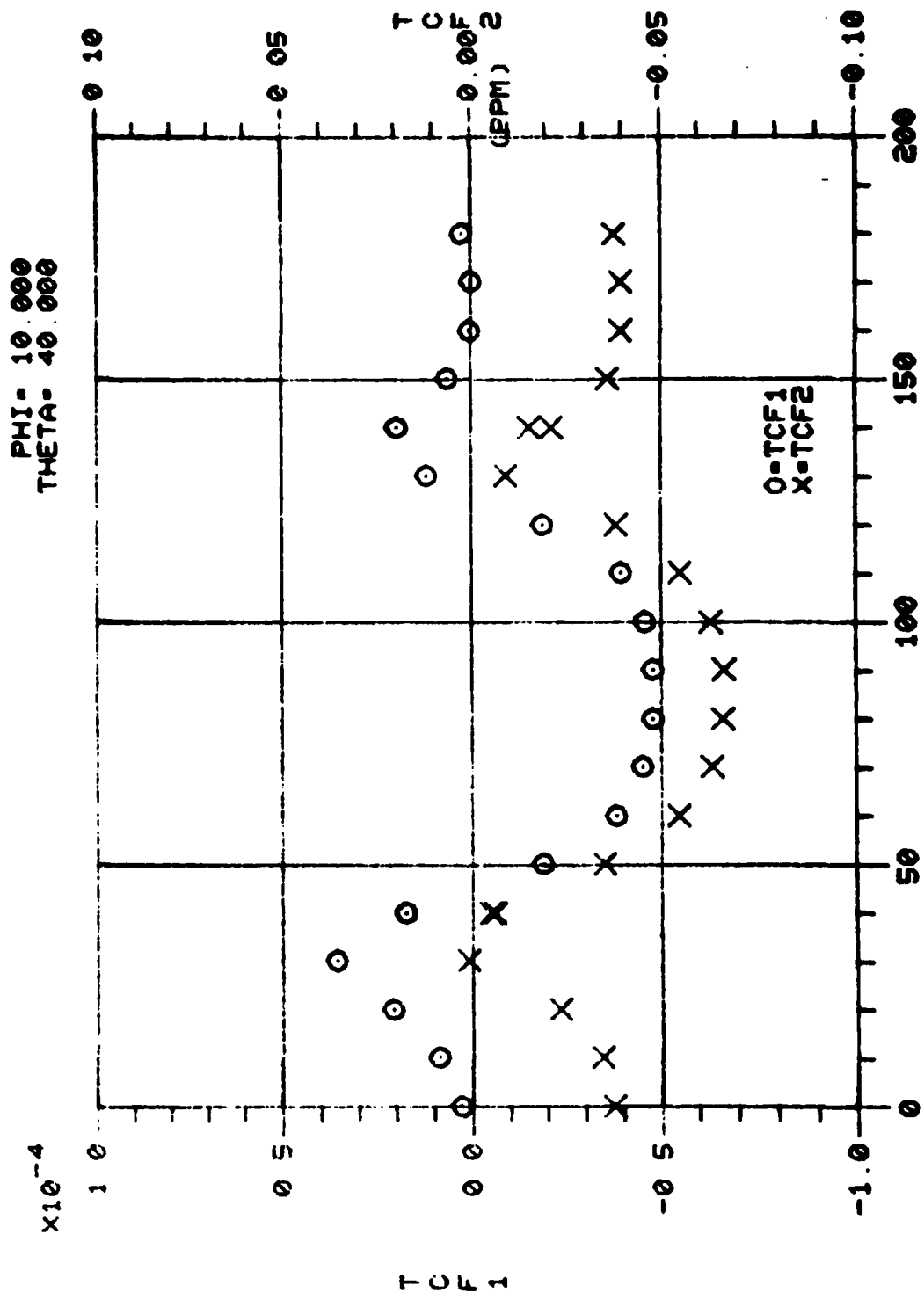
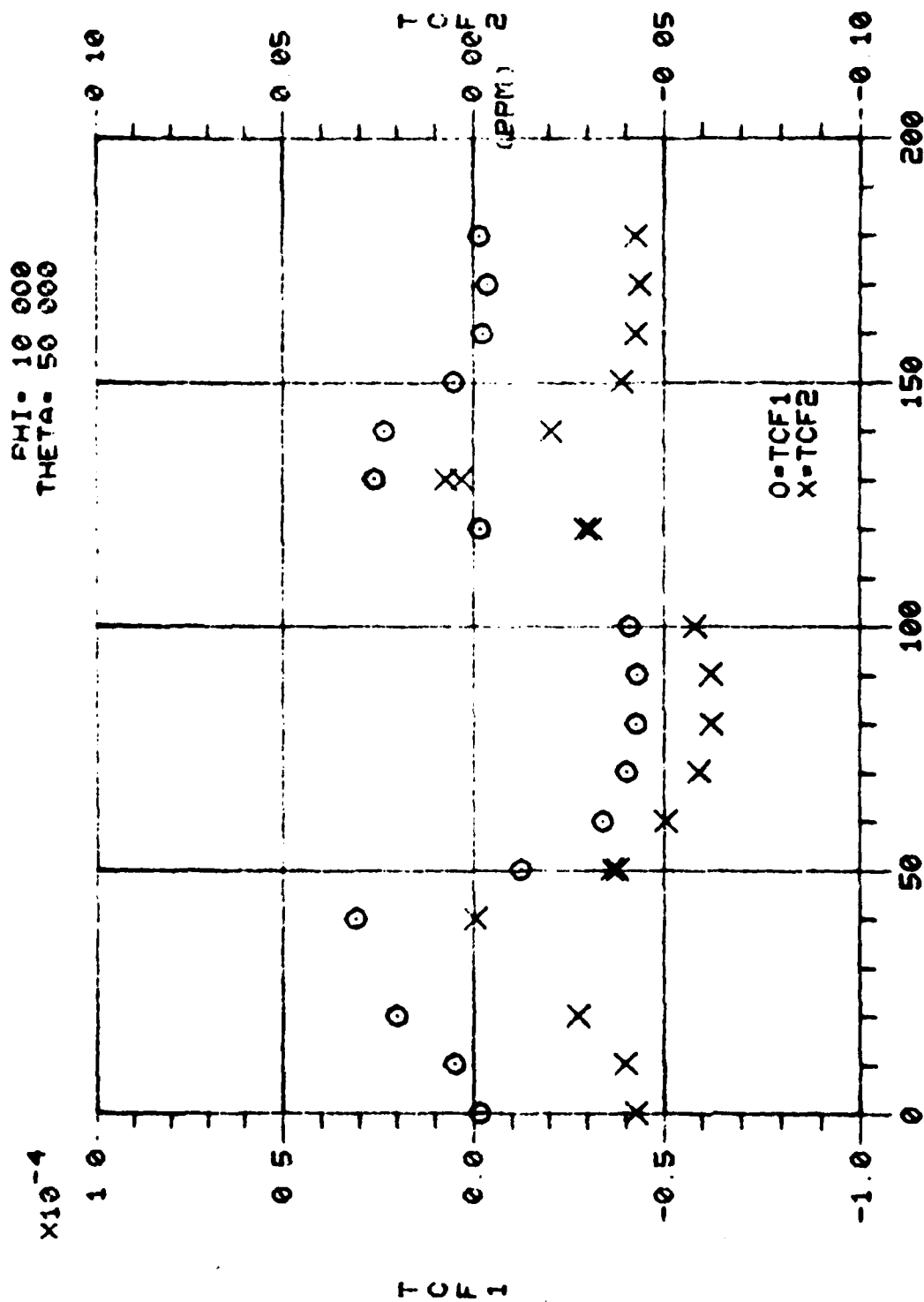


Figure 40. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles



PSI
 Figure 4P. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

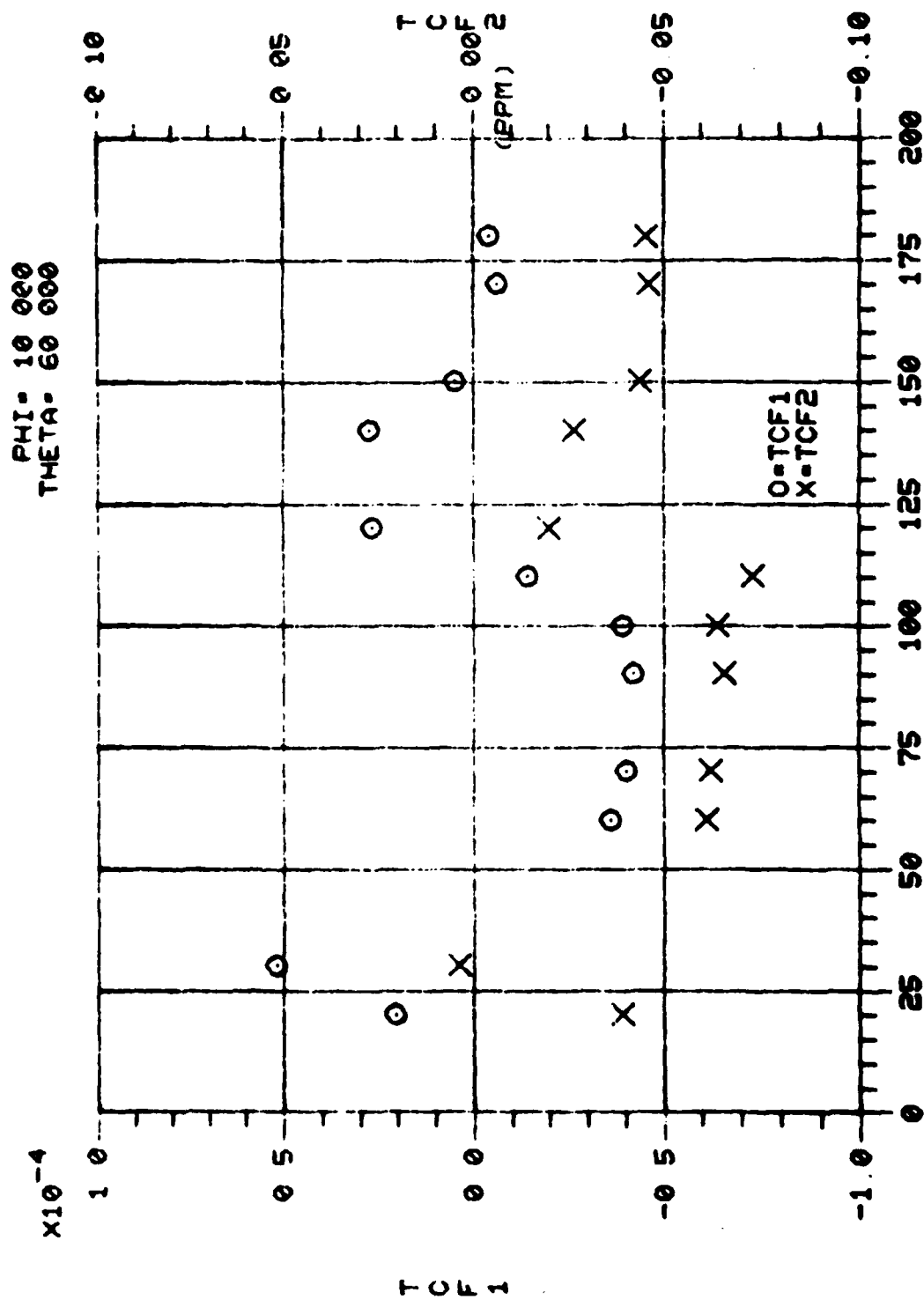


Figure 40. Calculated Values of TCF^{III} Versus Propagation Angles

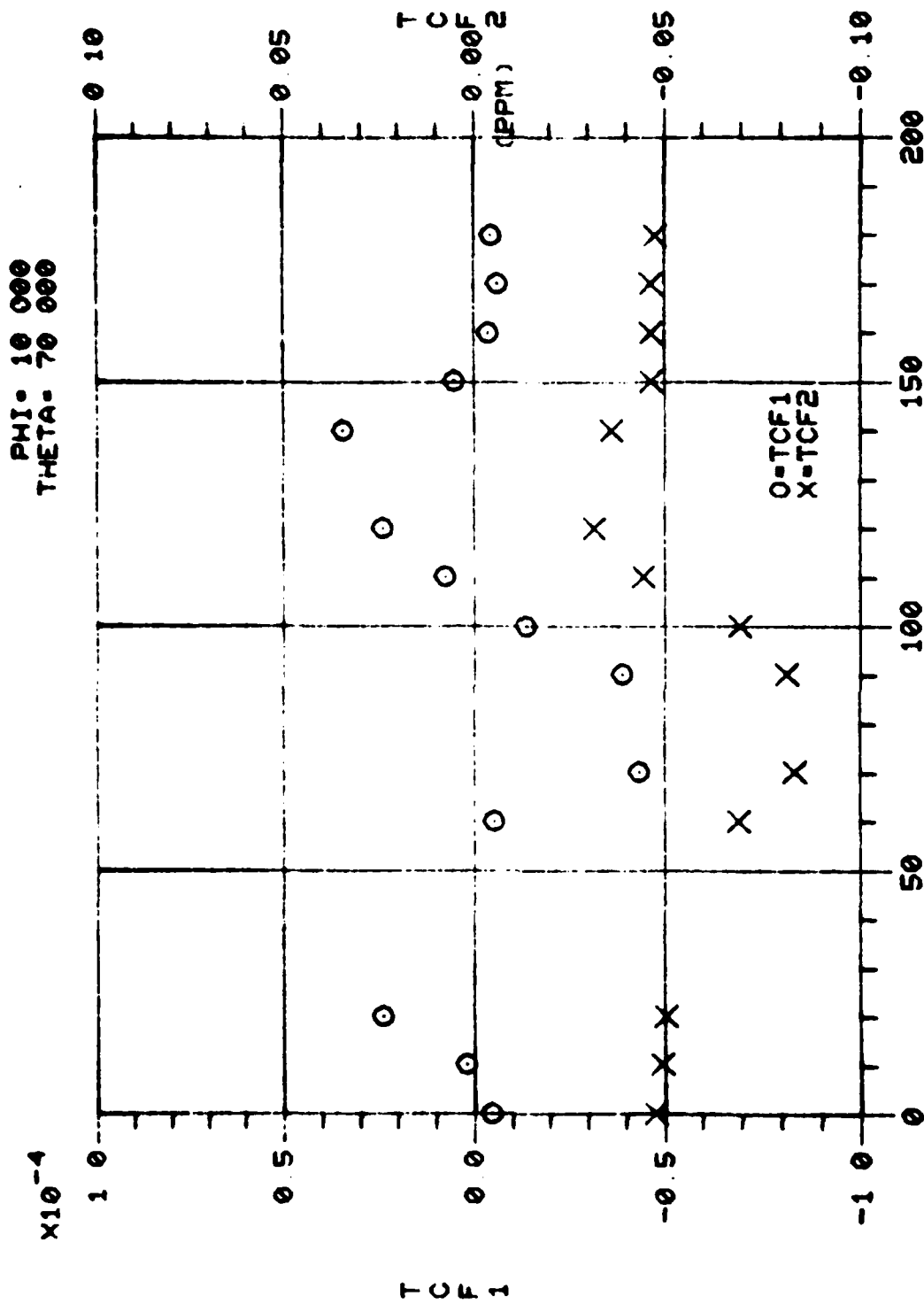


Figure 4R. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

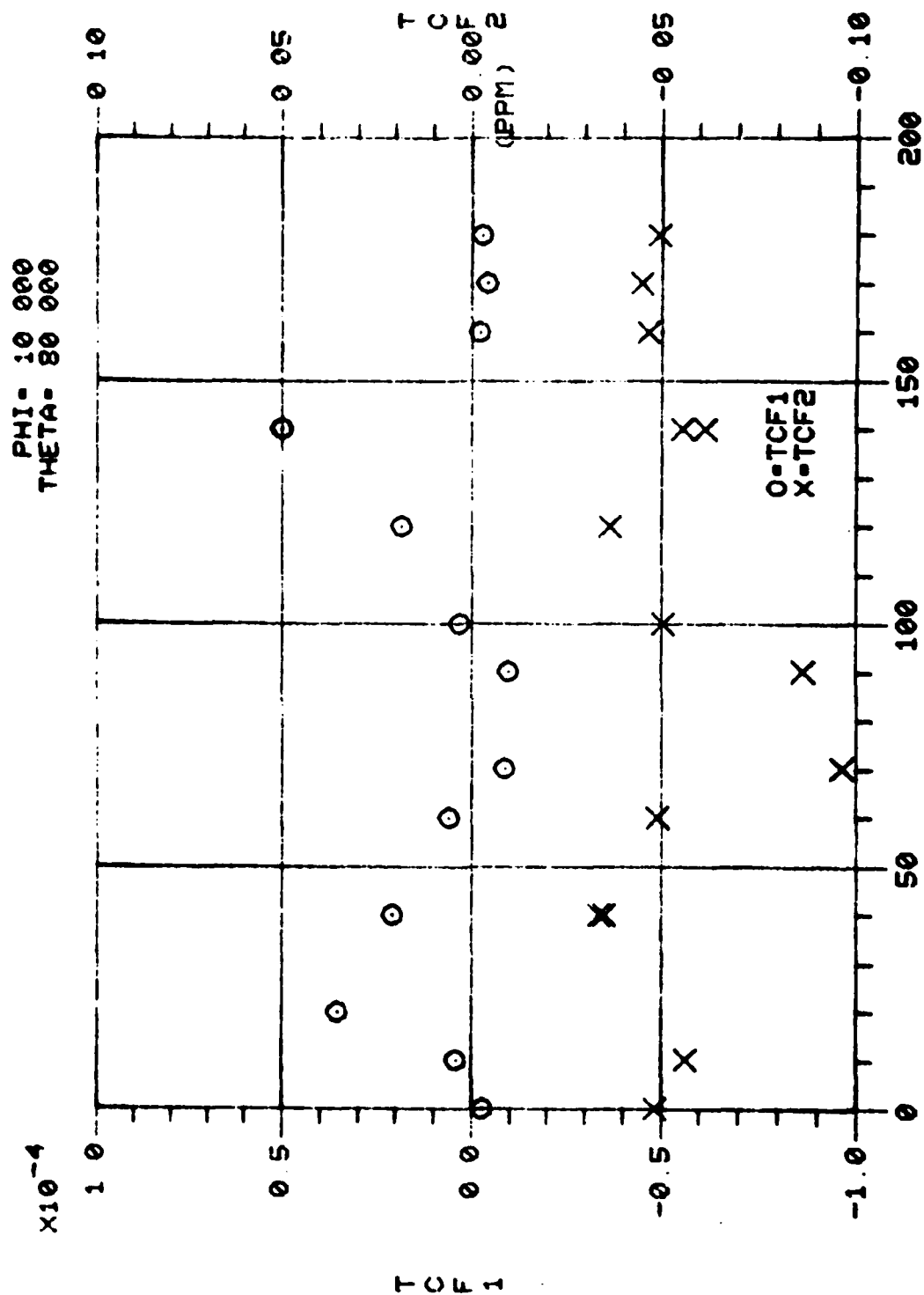


Figure 4S. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

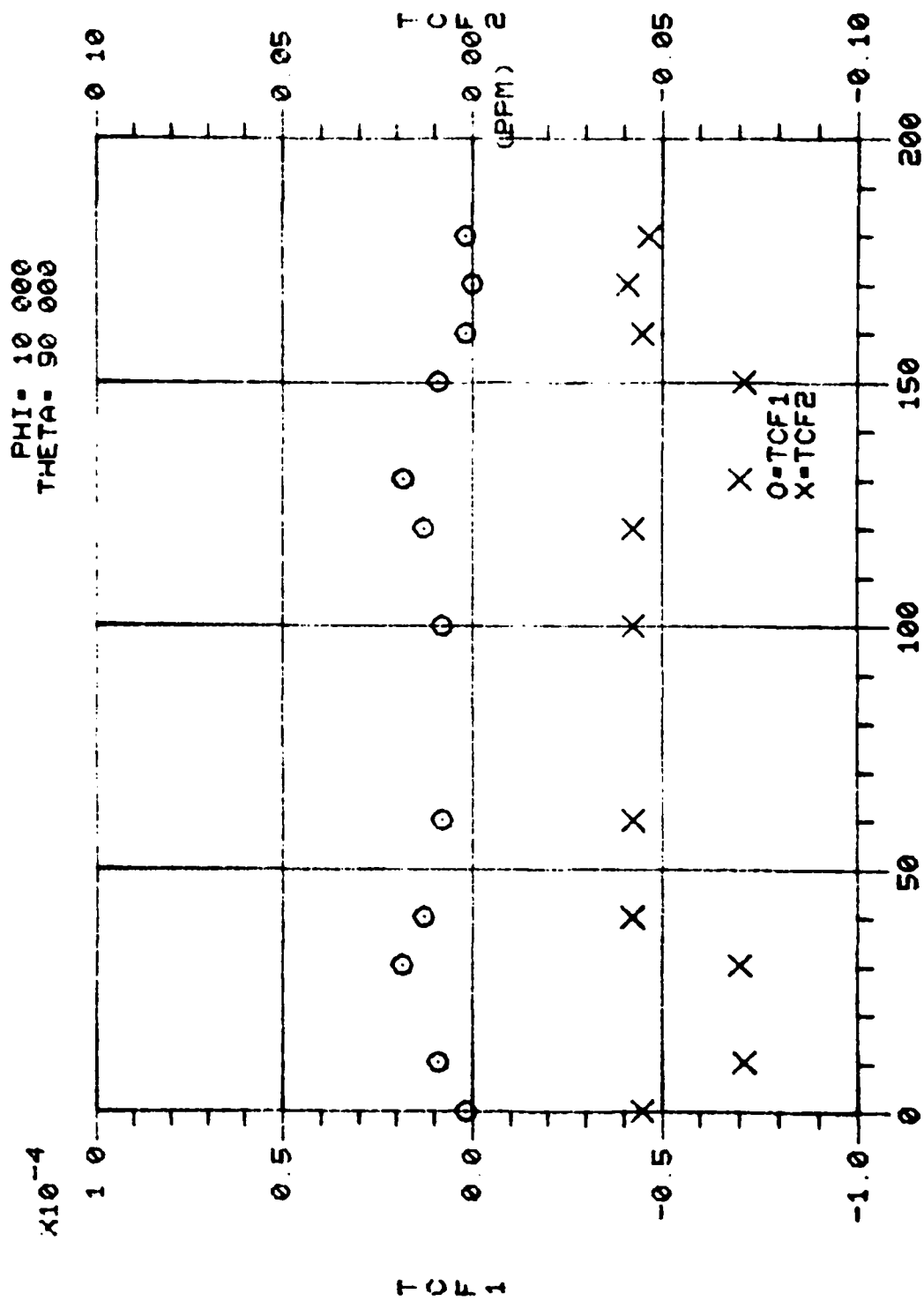


Figure 4T. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

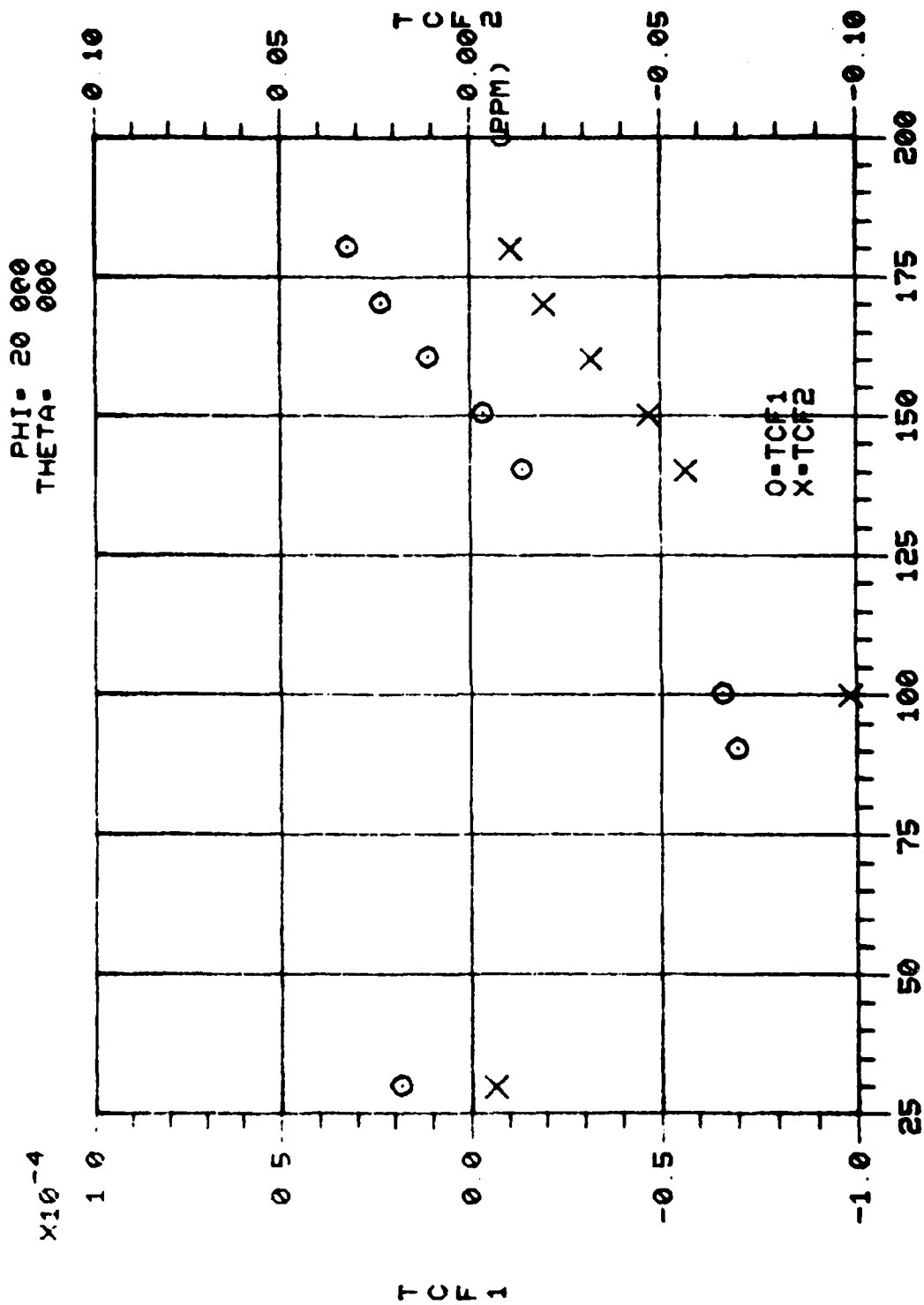


Figure 4U. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

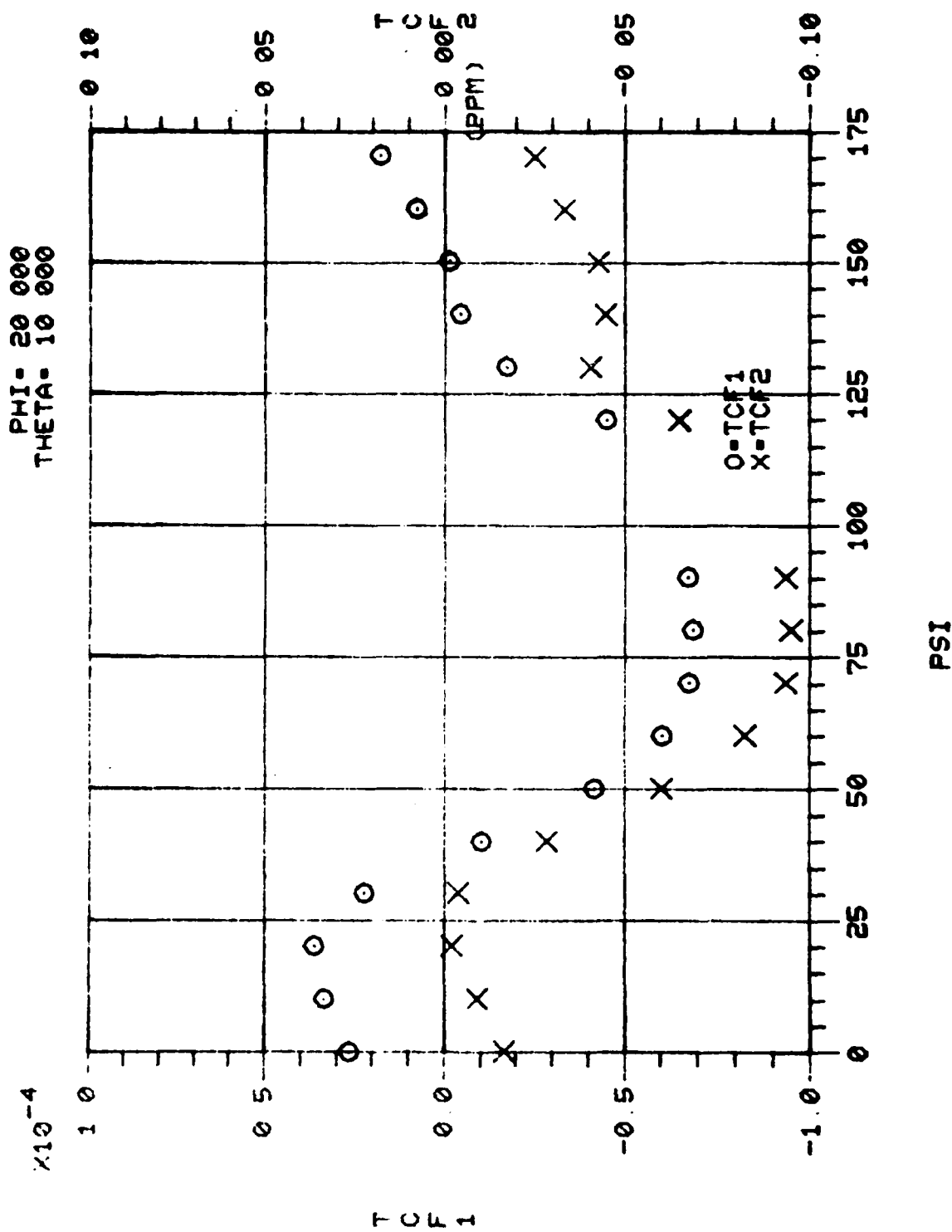


Figure 4V. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

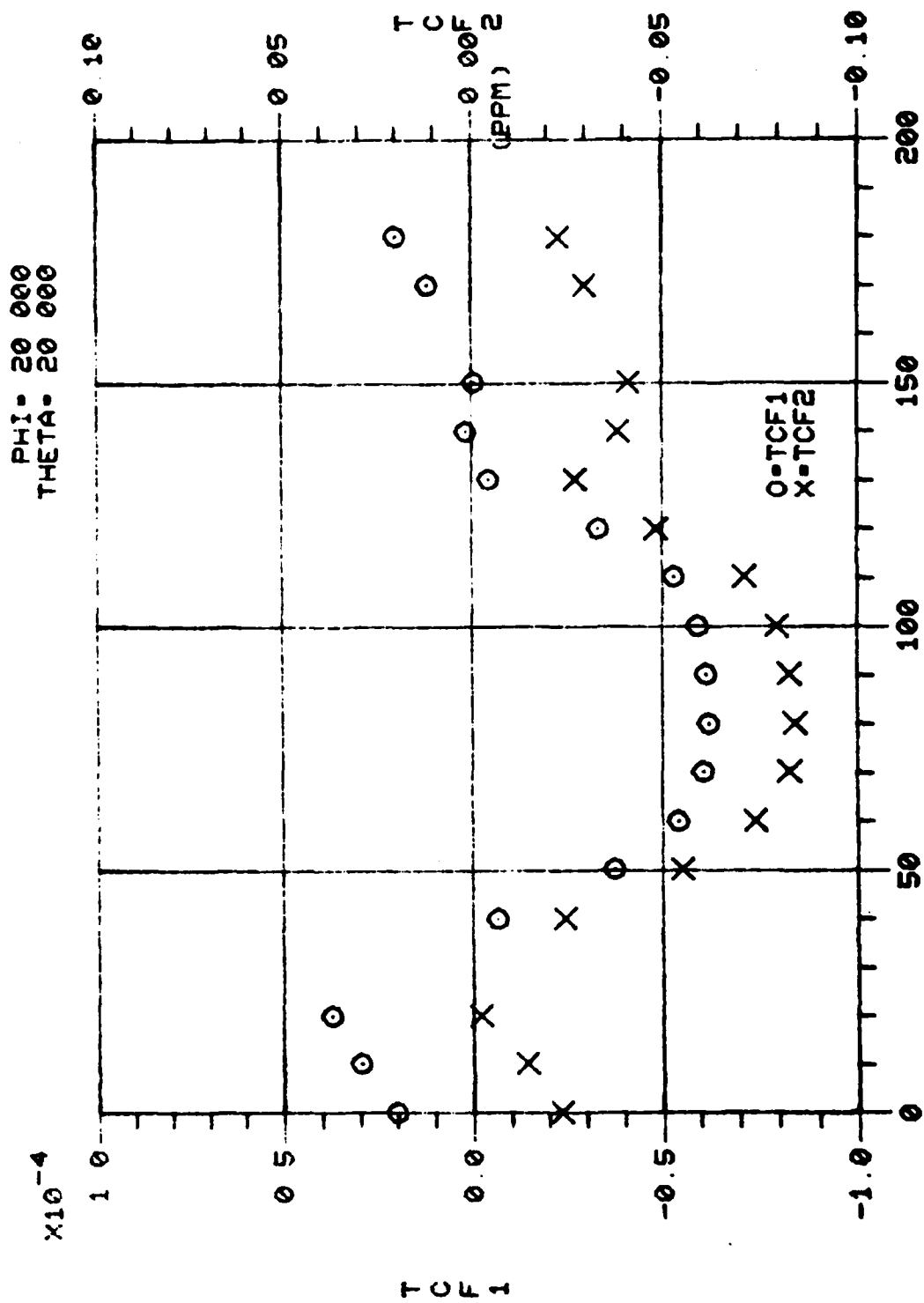


Figure 4W. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

PHI = 20.000
THETA = 30.000

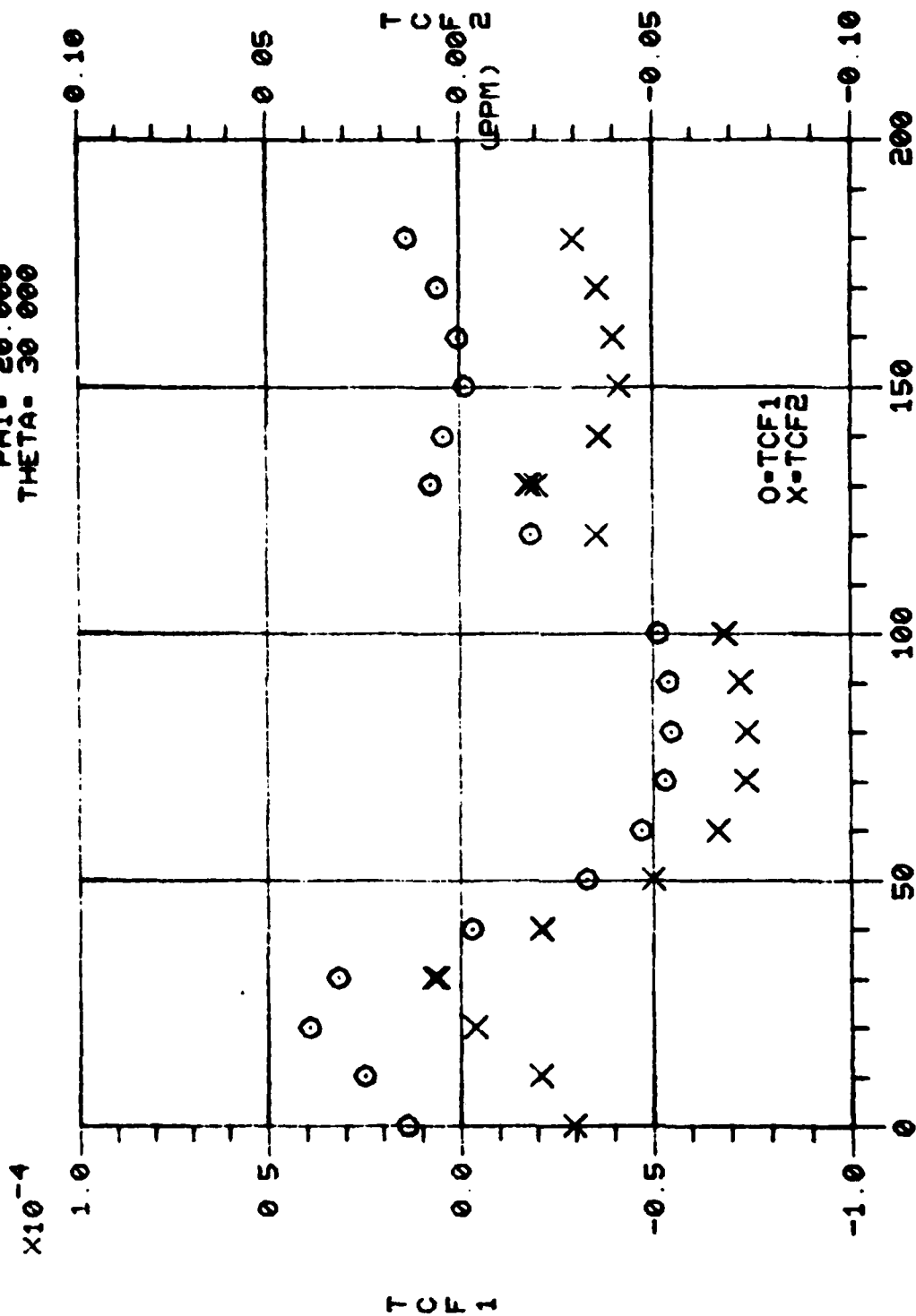


Figure 4X. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

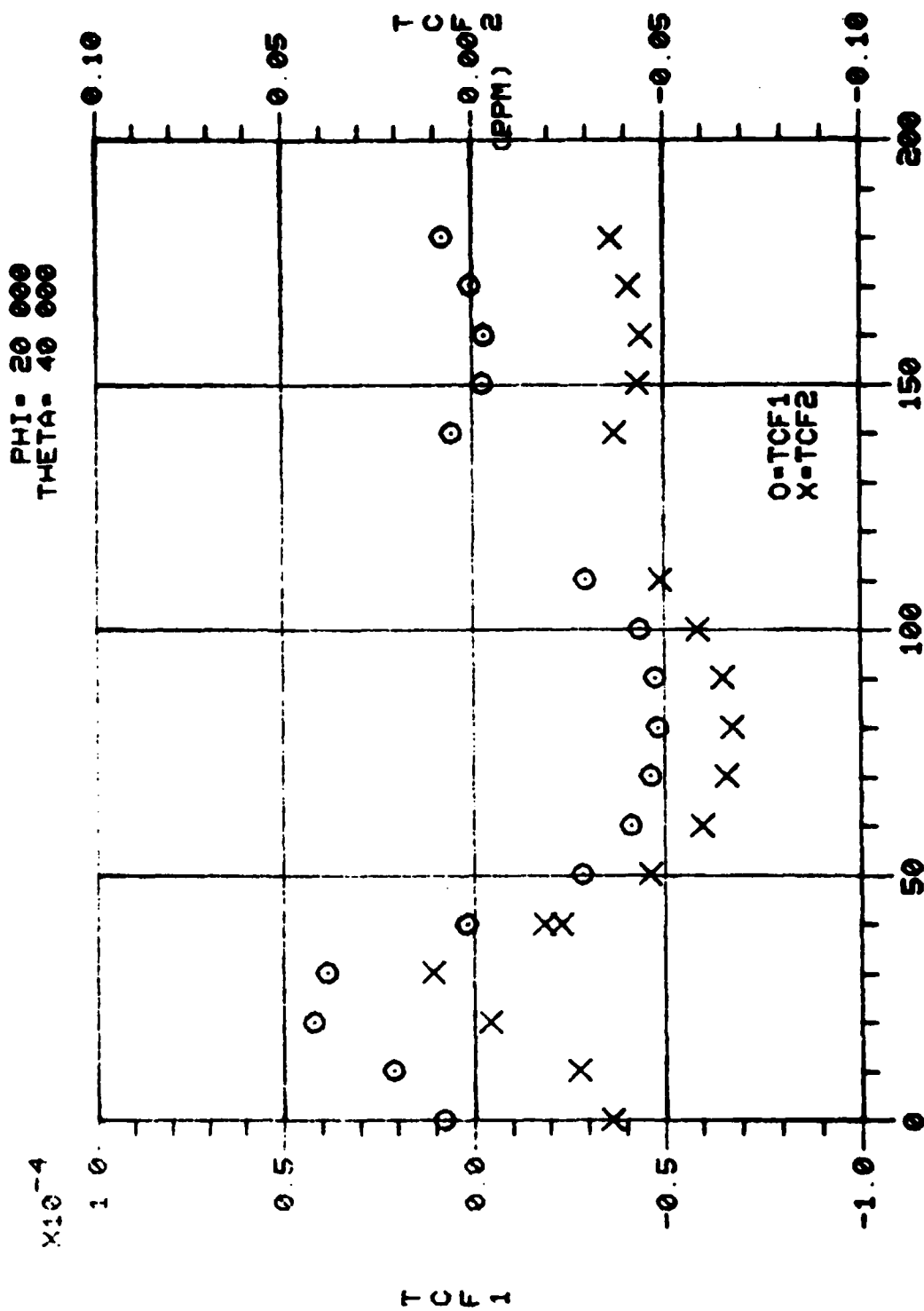


Figure 4Y. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

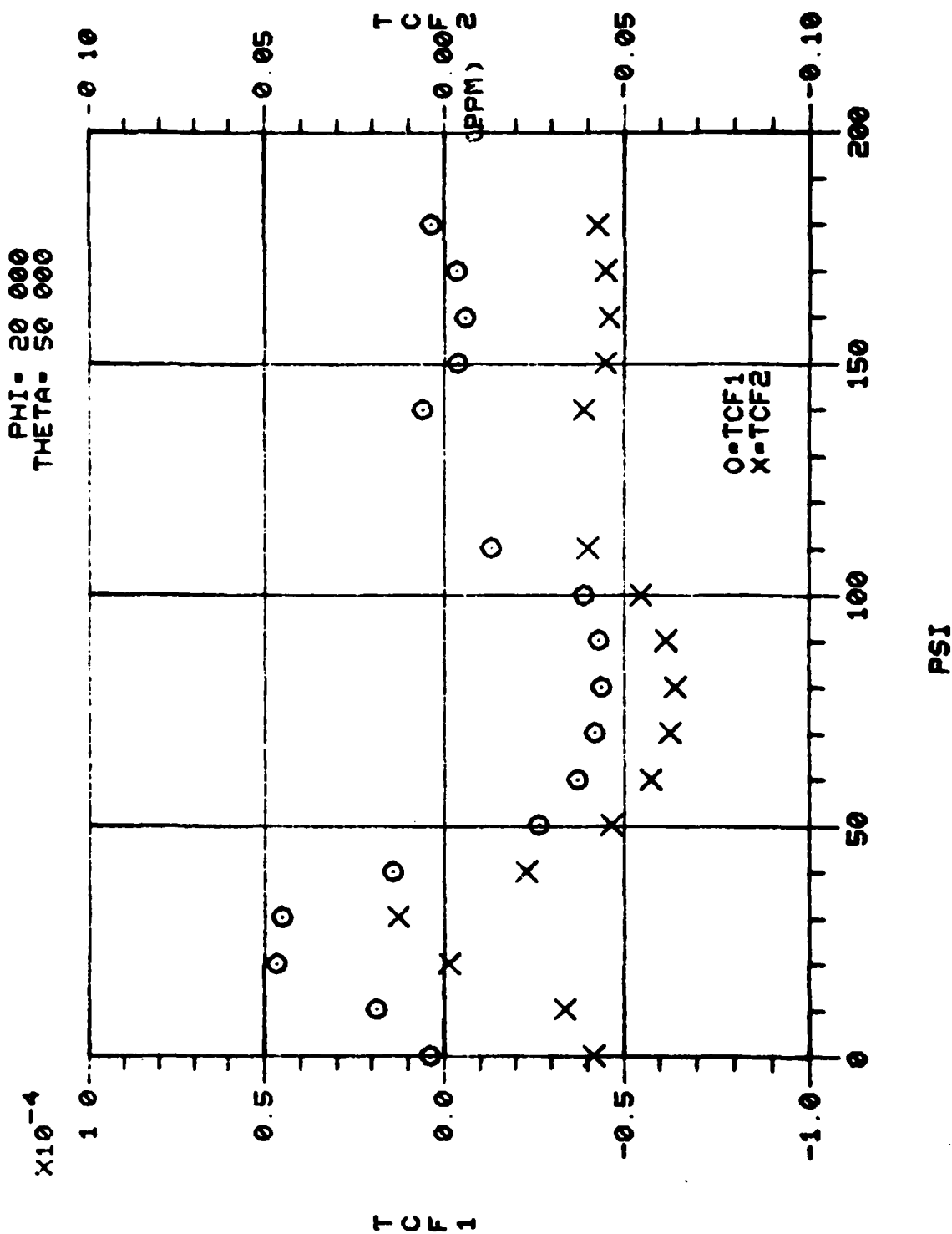


Figure 4Z. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

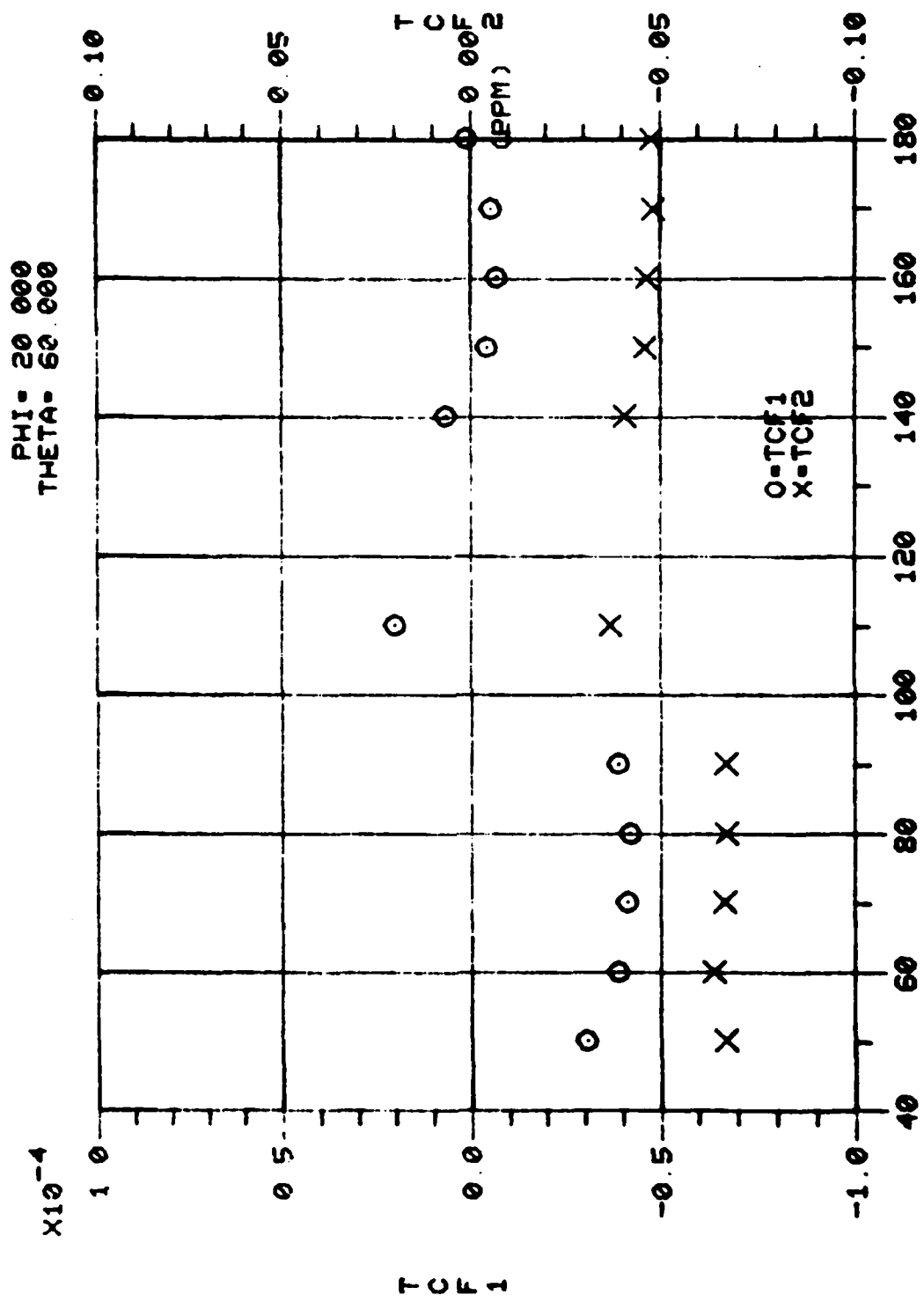


Figure 4AA. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

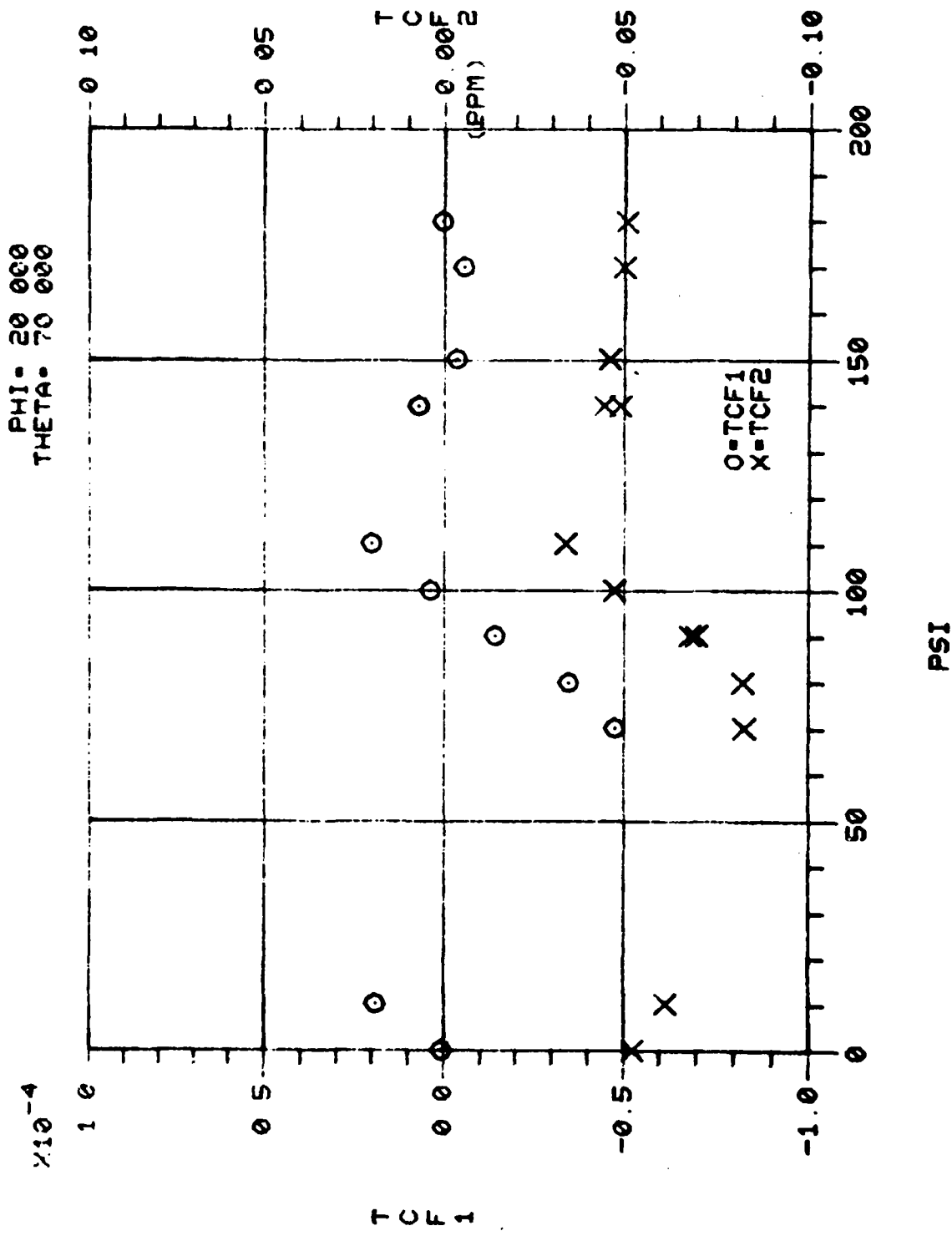


Figure 4BB. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

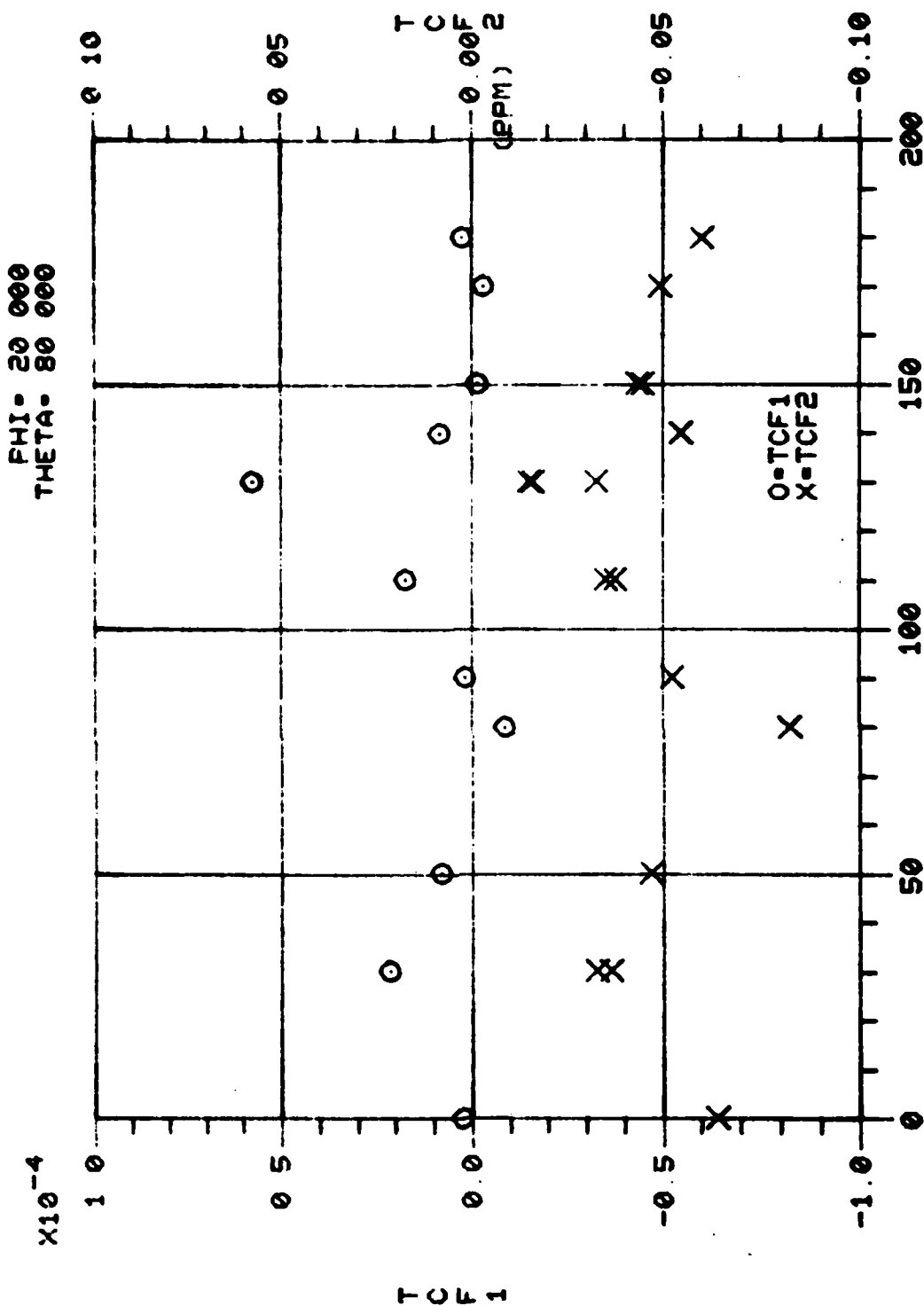


Figure 4CC. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

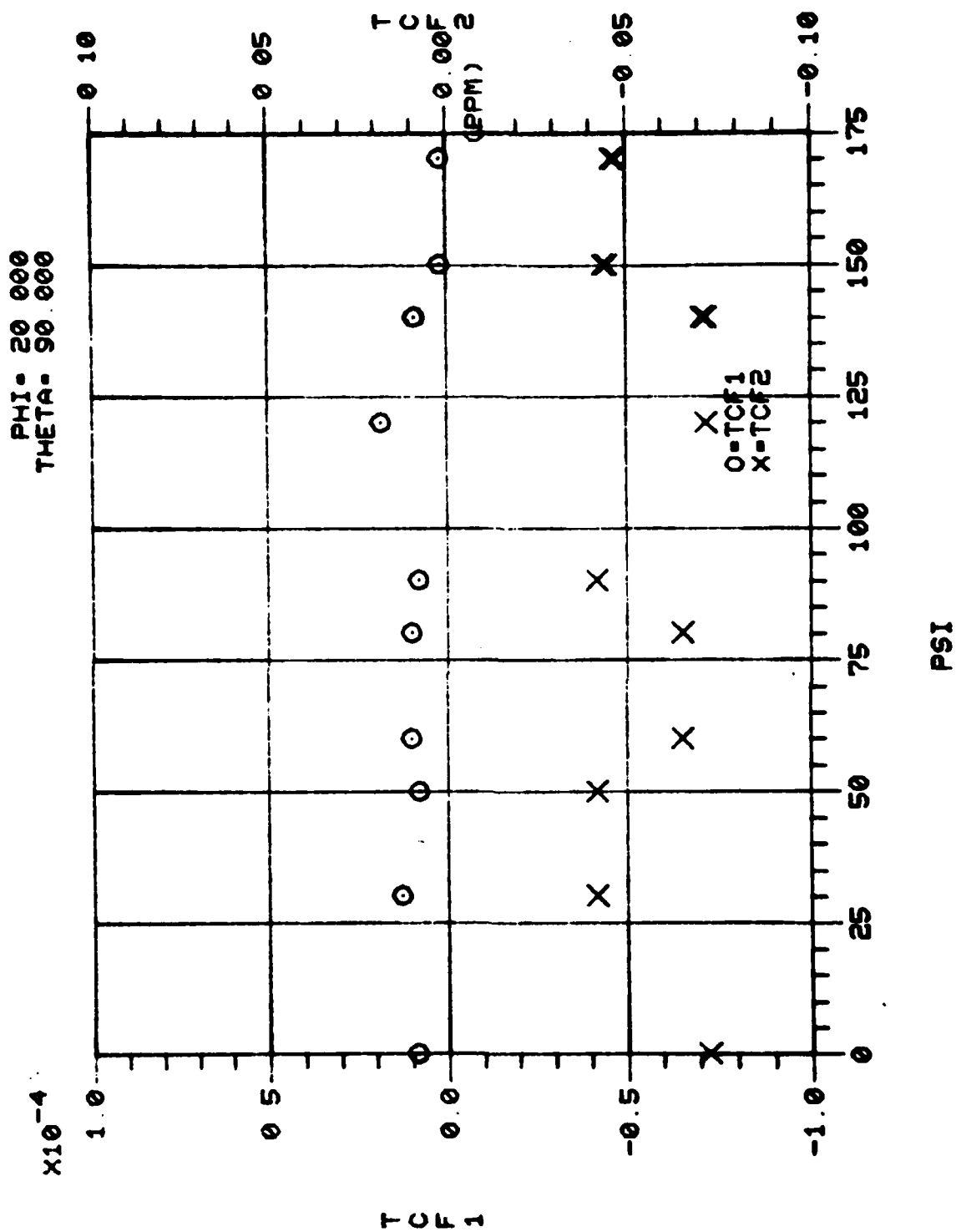


Figure 4DD. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

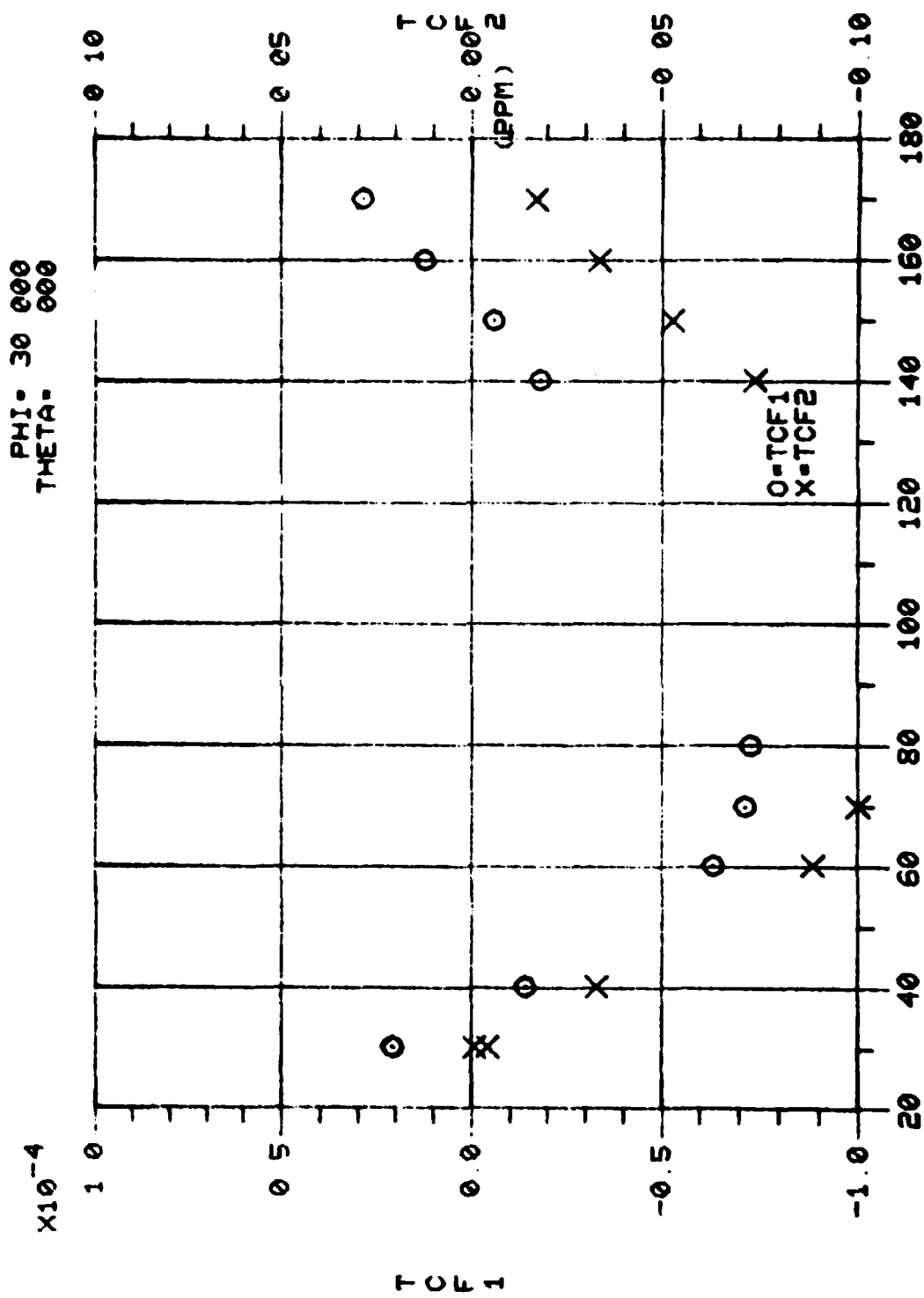


Figure 4EE. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

PHI- 30 000
 THETA- 10 000

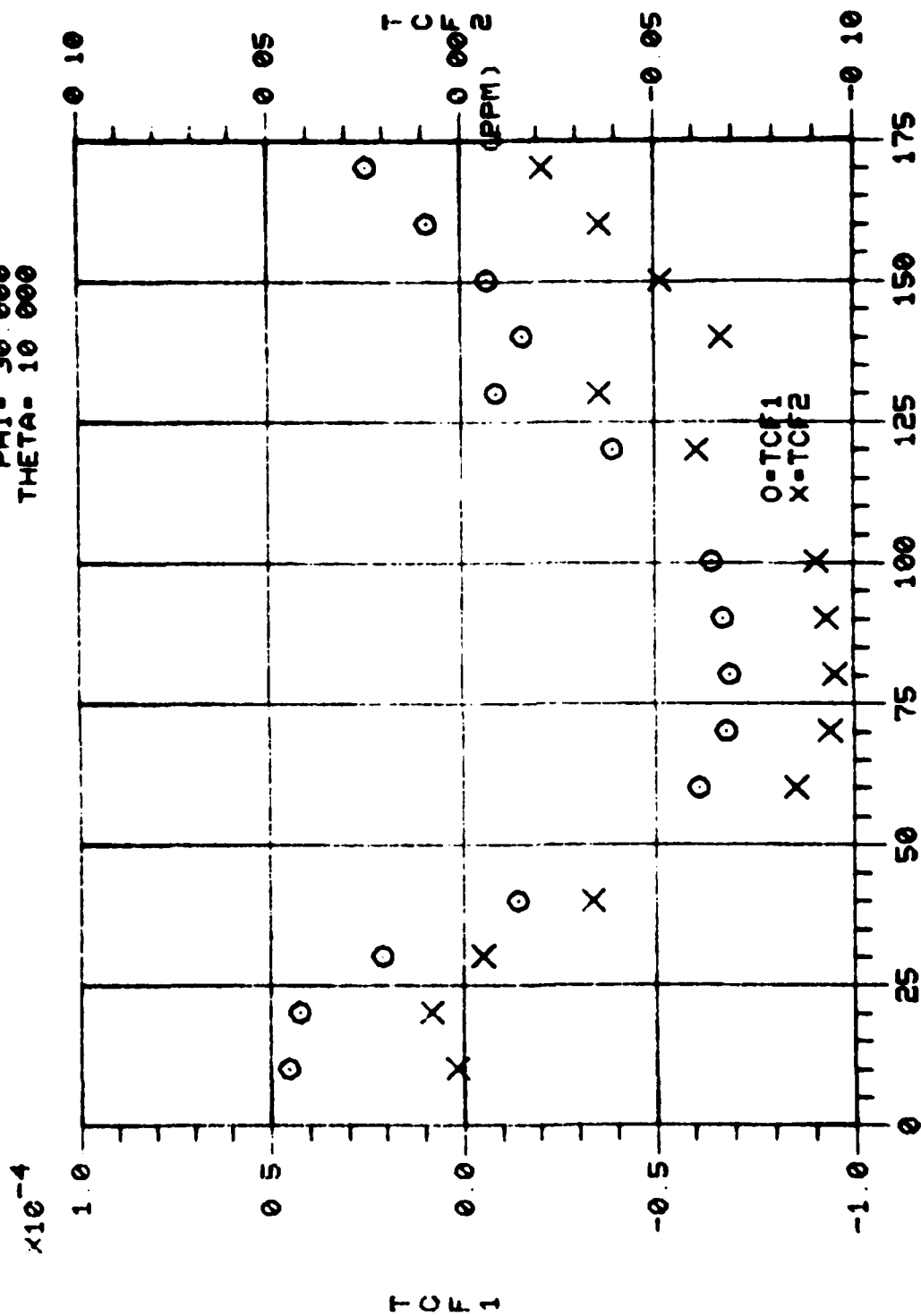


Figure 4FF. Calculated Values of $TCF^{(1)}$ Versus Propagation Angles

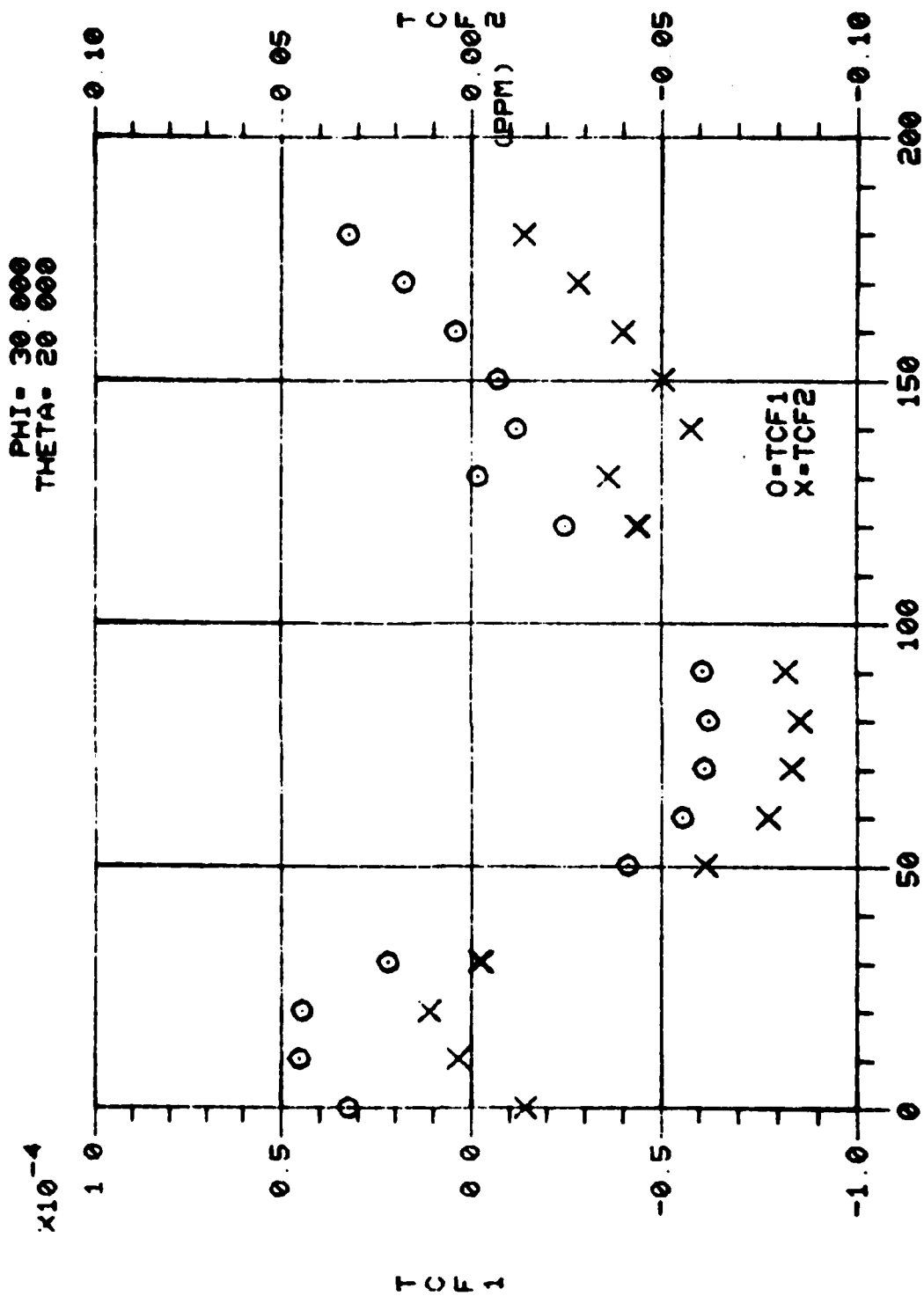


Figure 4GG. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

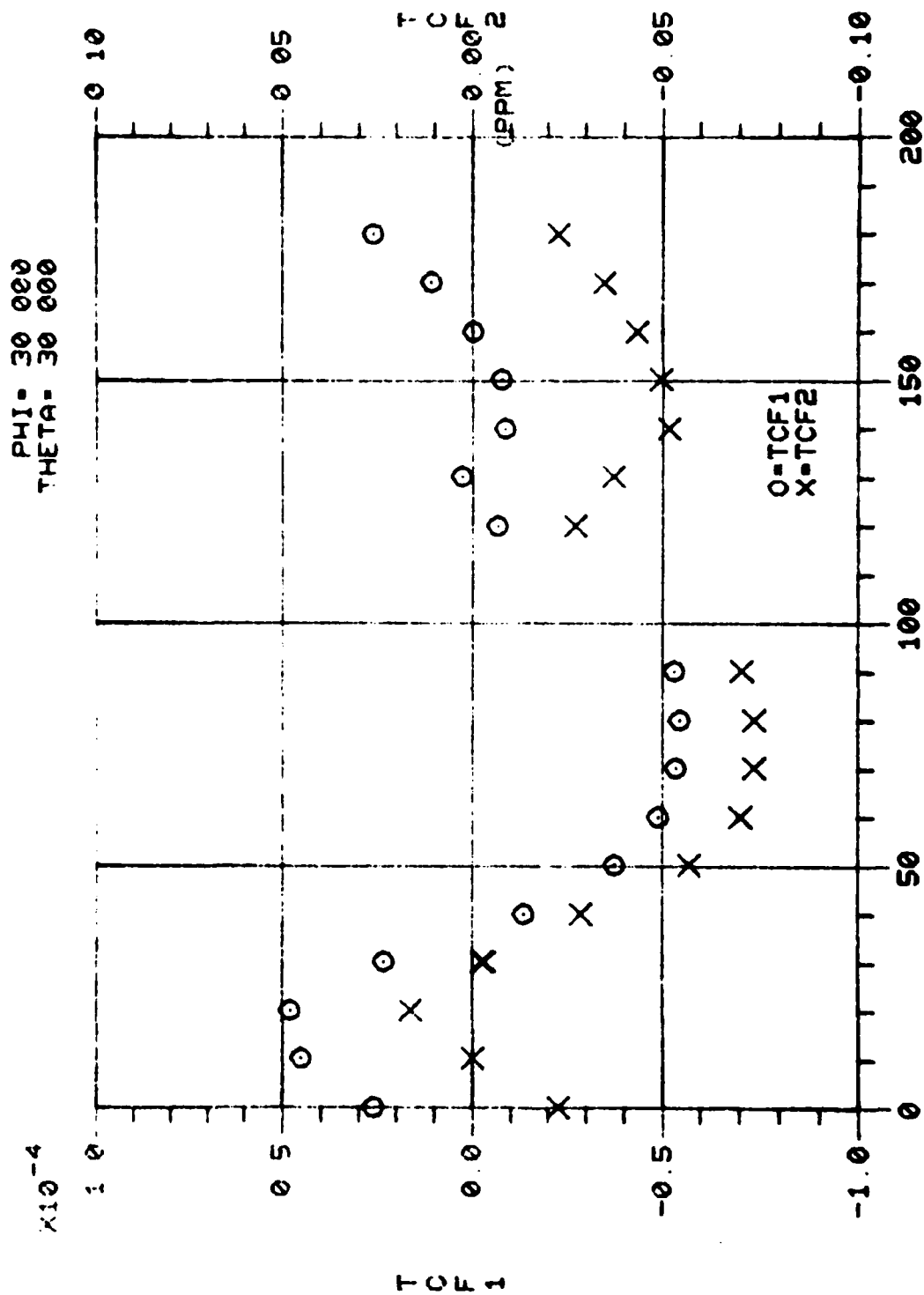


Figure 4HH. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

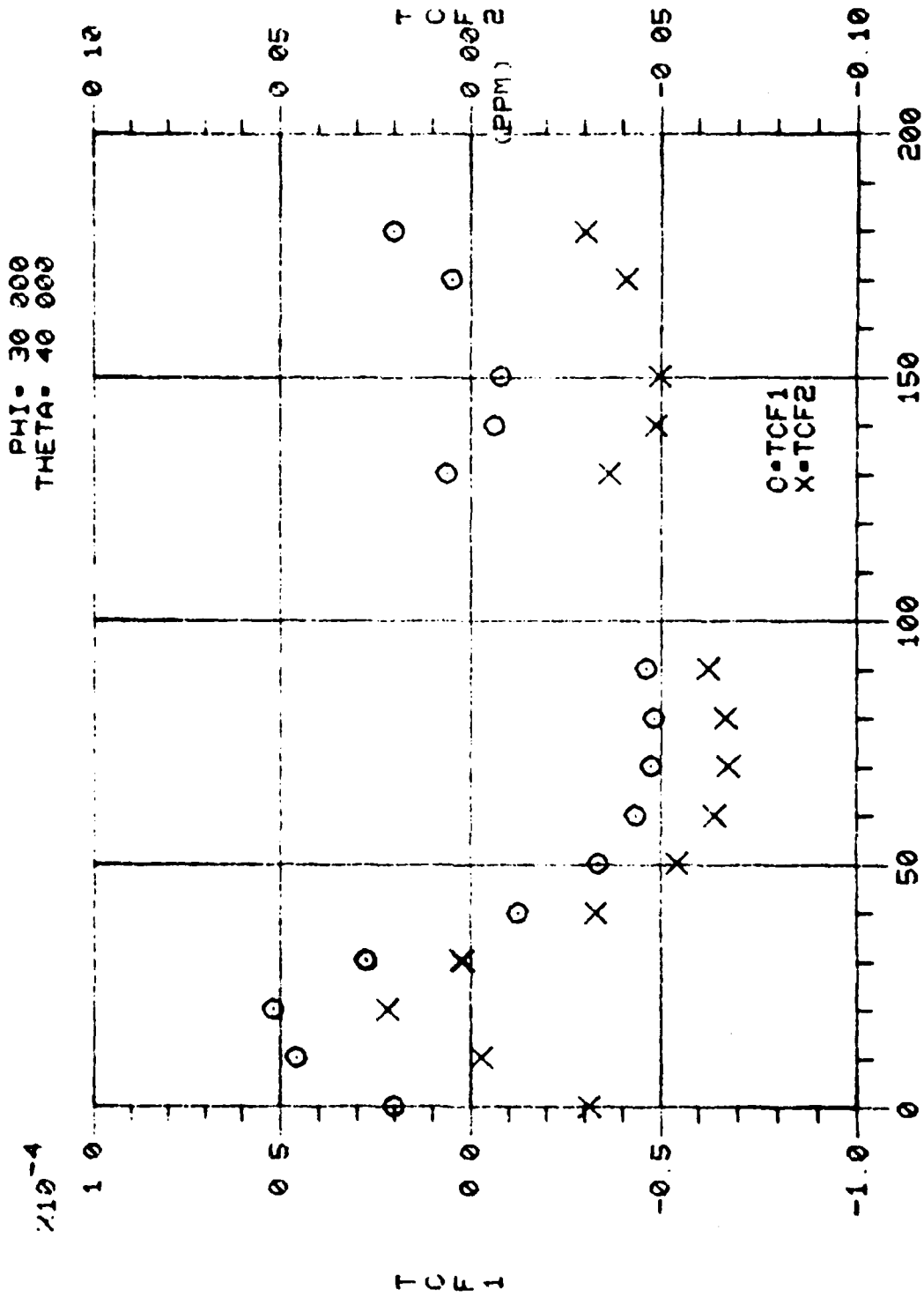


Figure 4II. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

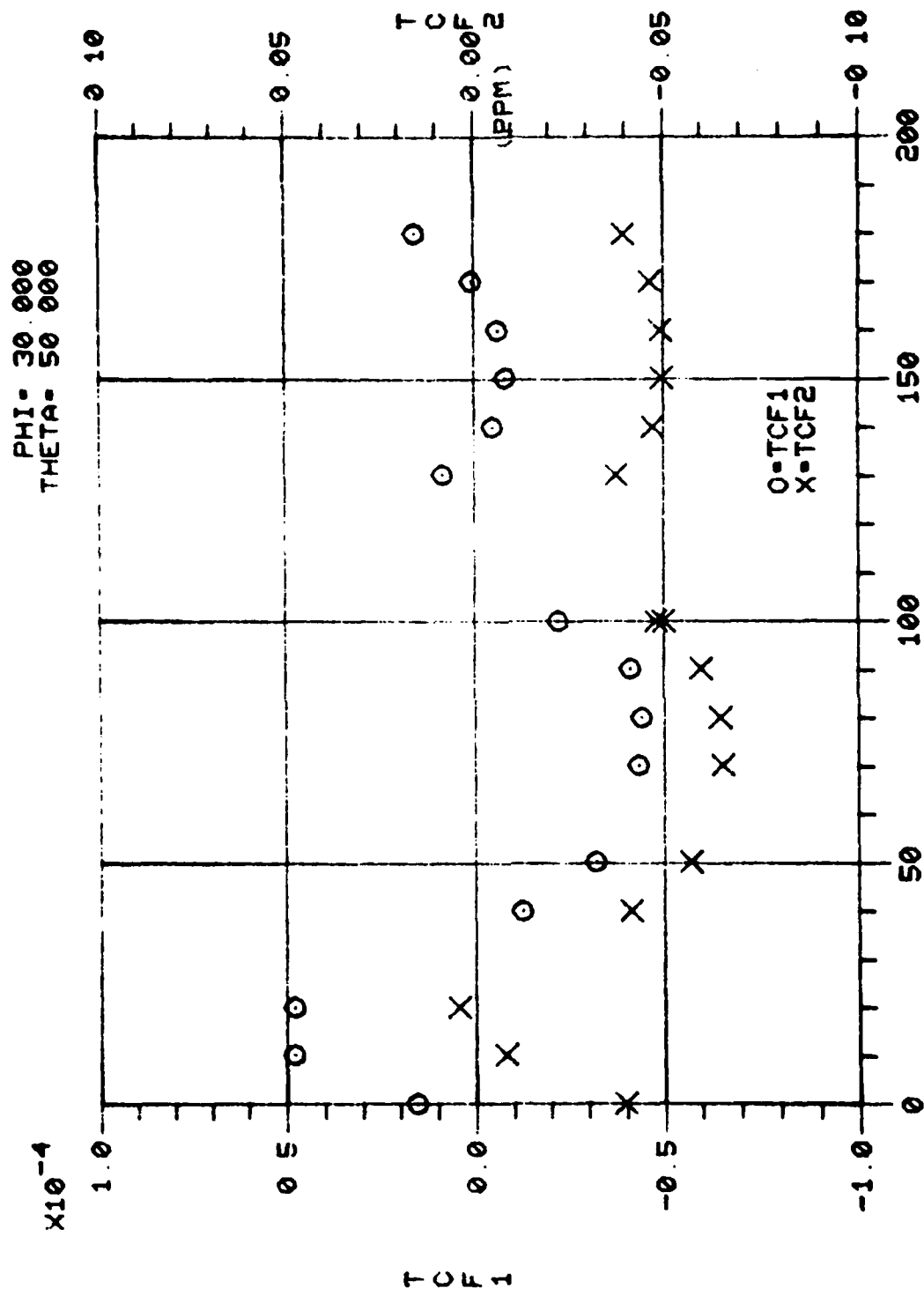


Figure 4JJ. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

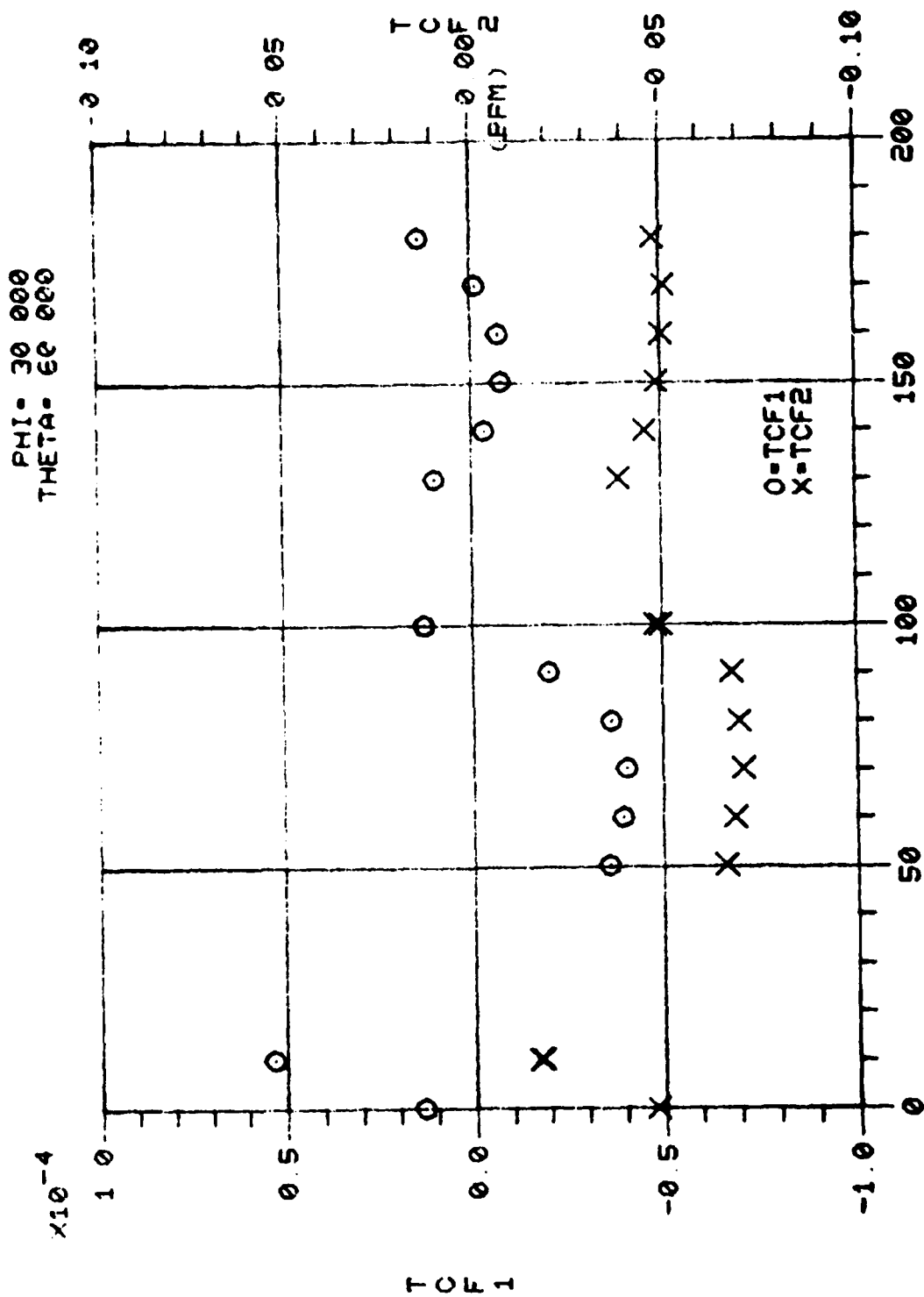


Figure 4KK. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

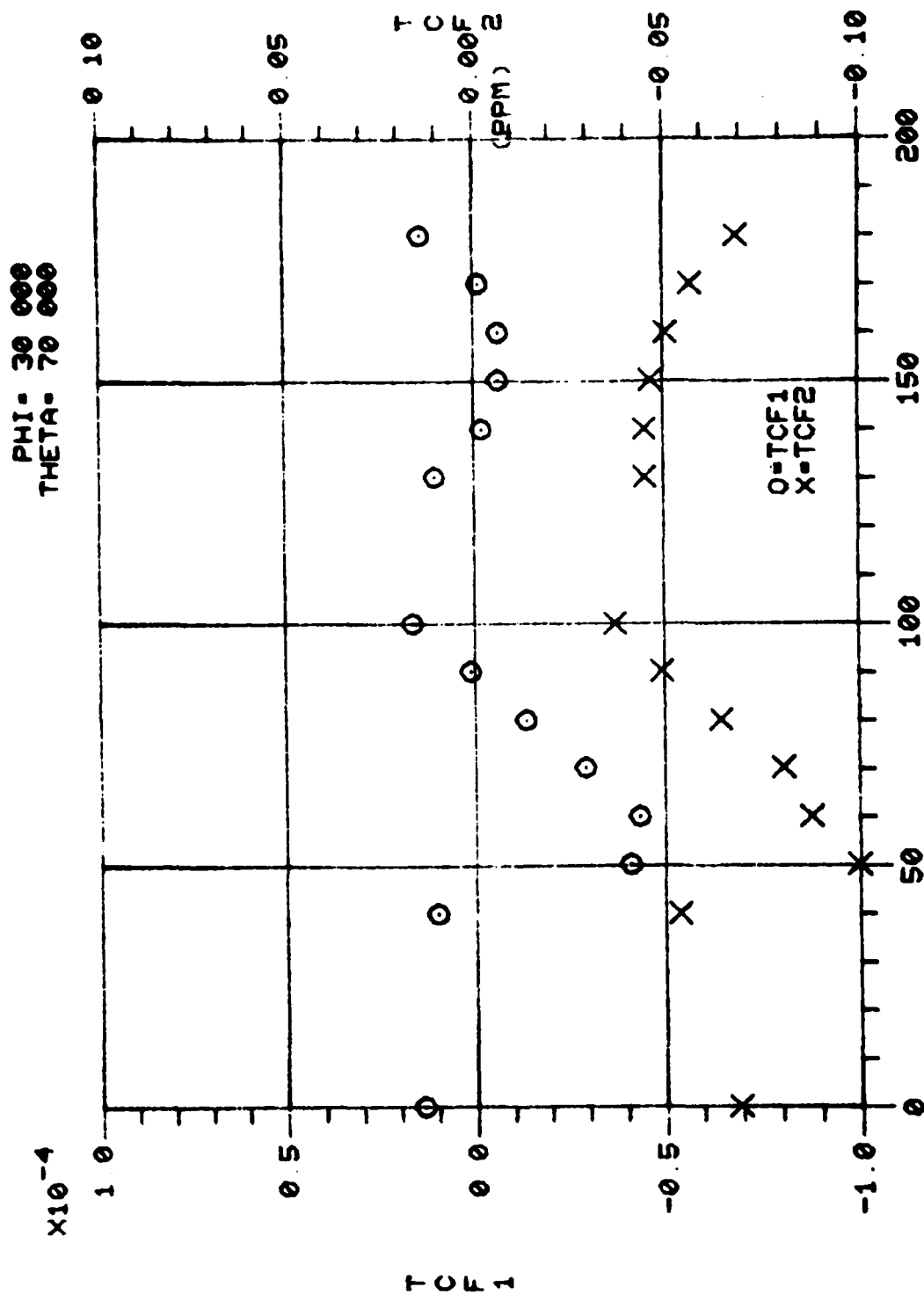
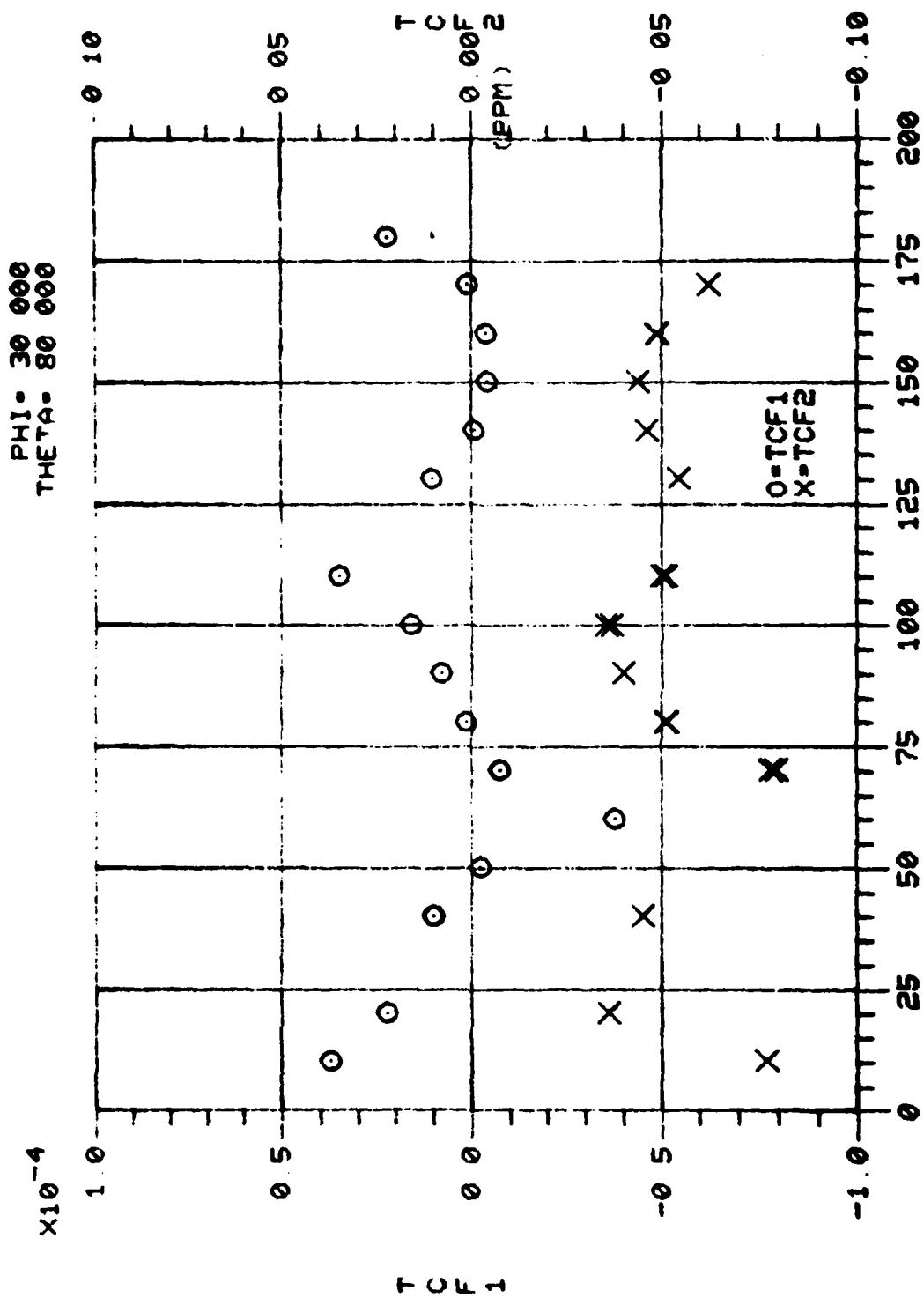


Figure 4LL. Calculated Values of TCF^{III} Versus Propagation Angles



PSI

Figure 4MM. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

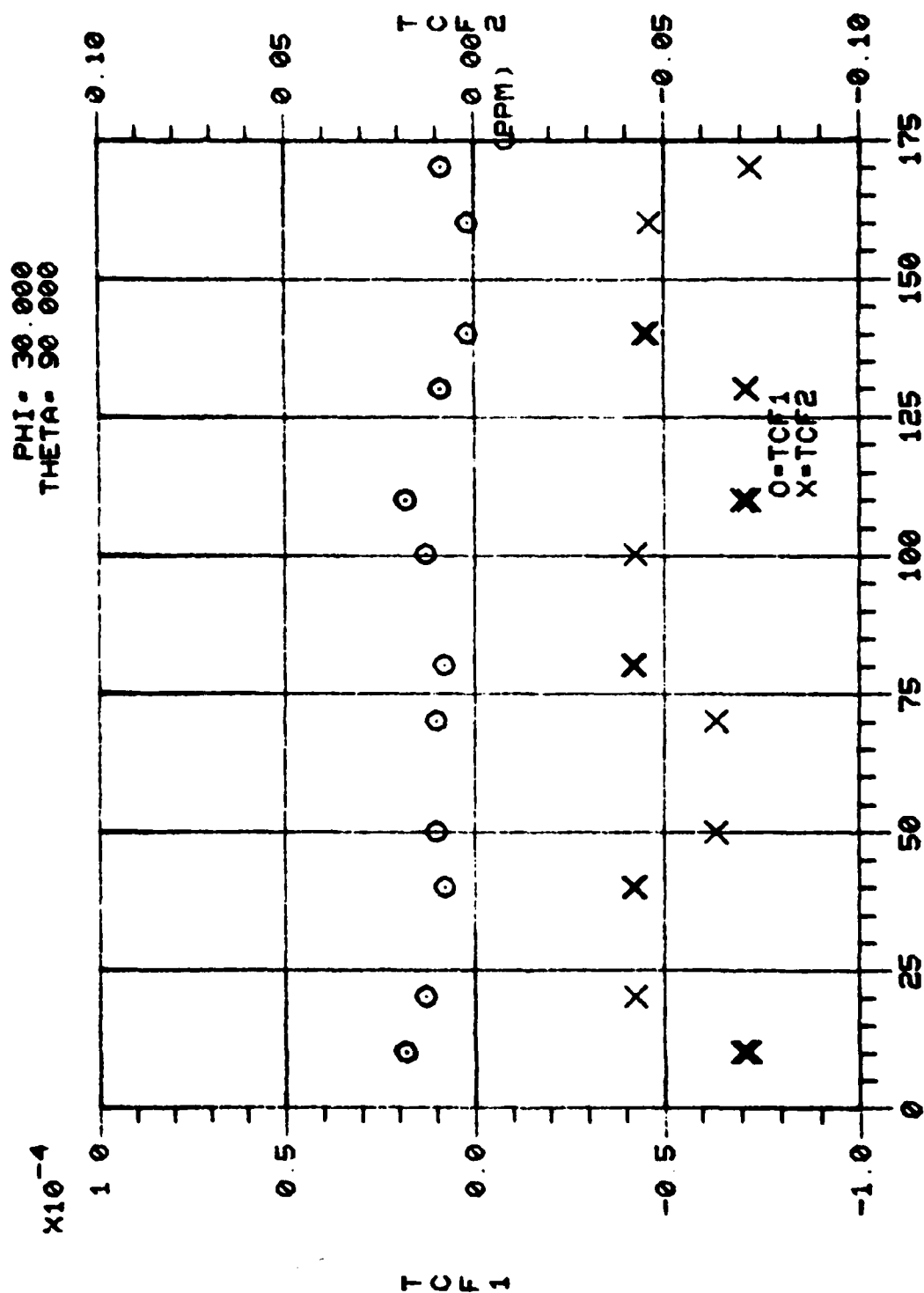


Figure 4NN. Calculated Values of TCF⁽¹⁾ Versus Propagation Angles

Calculations were performed on a $10^\circ \times 10^\circ \times 10^\circ$ grid over the angular ranges $0 \leq \text{PHI} \leq 30^\circ$, $0 \leq \text{PSI} \leq 180^\circ$, and $-90^\circ \leq \text{THETA} \leq 90^\circ$. These angular ranges, due to the symmetry of quartz, include all possible angular orientations. These initial calculations defined the "angular volumes" of low TCF orientations. Calculations were then performed on a $2.5^\circ \times 2.5^\circ \times 2.5^\circ$ grid near promising orientations. In this way, the entire angular range was explored and a large computer-based data file built. Maps of first and second order TCF's are shown in Figure 5. Zero first order TCF contours are drawn. In addition, contours of the second order TCF are drawn. In addition, contours of the second order TCF are drawn and shaded in areas where the second order TCF is less than $0.01 \text{ PPM}/^\circ\text{C}^2$. This represents a substantial improvement over ST quartz, for which the second order for TCF is approximately $0.03 \text{ PPM}/^\circ\text{C}^2$. Where data points were missing, lines were connected by interpolation.

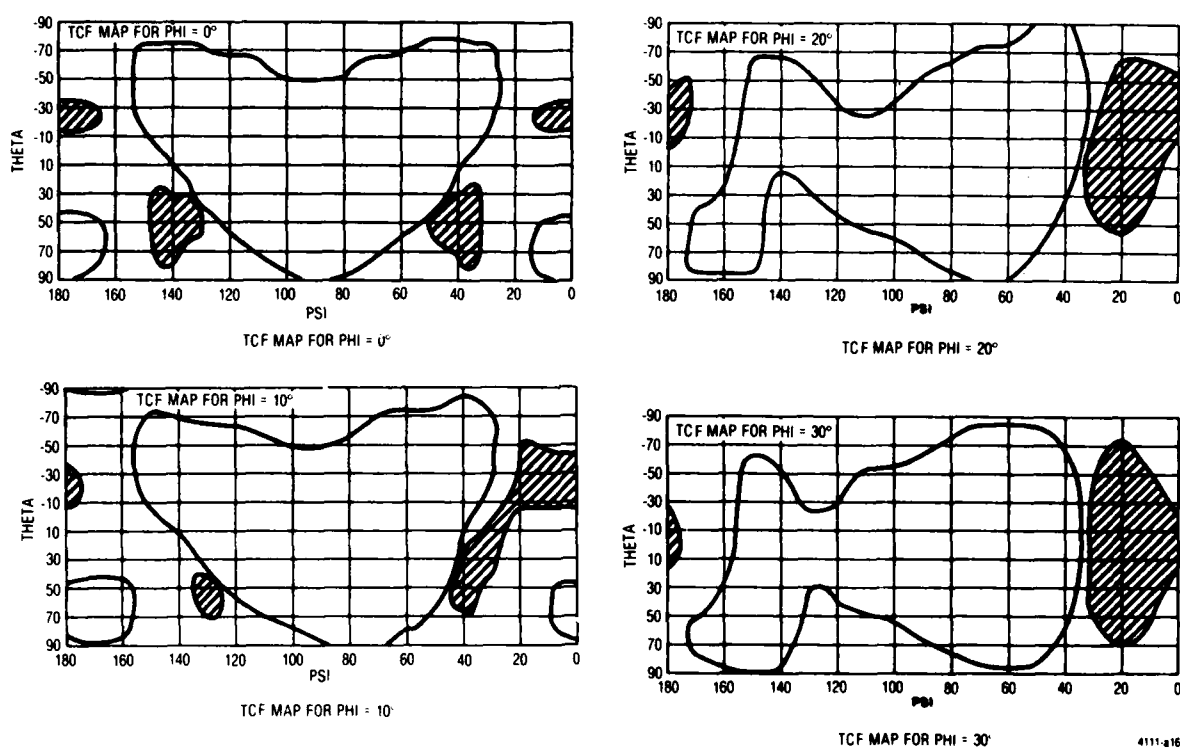


Figure 5. TCF Map of SAW Device on Quartz

Despite the number and density of points at which the first and second order TCFs were calculated, wherever $\text{TCF}^{(1)}$ was found to be less than or equal to zero, we found $\text{TCF}^{(2)}$ to be less than 0. The reason for this probably lies in the lack of independence of the crystal constants themselves. Using the volume perturbation approach of Auld¹, one obtains equation A-8 of Appendix A.

¹"Acoustic Fields and Waves in Solids," Auld, B. A., Vol. II, John Wiley & Sons, 1973, N. Y., p. 297.

For small changes in ρ and $c^{(0)}$, one might expect that the TCFs are well correlated with the temperature derivatives of the fundamental constants for Rayleigh waves in quartz. A list of some of the crystal elastic constants¹¹ temperature derivatives is in Table 1.

TABLE 1. CRYSTAL ELASTIC CONSTANTS' TEMPERATURE DERIVATIVES

	TC ⁽¹⁾	TC ⁽²⁾	TC ⁽³⁾
C ₁₁	-48.5×10^{-6}	-107×10^{-9}	-70×10^{-12}
C ₁₂	-3000	-3050	-1260
C ₁₃	-550	-1150	-750
C ₁₄	101	-48	-590
C ₃₃	-160	-275	-250
C ₄₄	-177	-216	-216
C ₆₆	178	118	21
ρ	-34.92	-15.9	5.3
α_{11}	13.7	6.5	-1.9
α_{33}	7.5	2.9	-1.5

Figure 6 shows a plot of these values. The correlation is quite high, except for the case of C₁₄ and suggests that the TCFs should be correlated also. Plots of TCF⁽¹⁾ and TCF⁽²⁾ versus angles shown in Figure 4A through 4NN reflect this correlation.

Of course, if the two TCF surfaces do not intersect to form a line of zero TCF⁽¹⁾ and TCF⁽²⁾, we must use a slightly different approach to finding temperature stable cuts. The largest variation in constants occurs for C₁₂. As we are interested in the temperature range from -50°C to 100°C, the maximum deviation of T from T₀ = 25°C is $|T - T_0| = 75^\circ\text{C}$. Calculating the changes in the constant C₁₂ for this maximum temperature change gives:

$$\frac{1}{C_{12}} \left| \Delta C_{12}^{(1)} \right| = 2.25 \times 10^{-1}$$

$$\frac{1}{C_{12}} \left| \Delta C_{12}^{(2)} \right| = 1.72 \times 10^{-2}$$

$$\frac{1}{C_{12}} \left| \Delta C_{12}^{(3)} \right| = 5.32 \times 10^{-4}$$

¹¹"Higher Order Temperature Coefficients of the Elastic Stiffnesses and Compliances of Alpha-Quartz", Bechmann, Ballato, Lukaszek, Proc. IRE, Aug 1962, pp. 1812-1922.

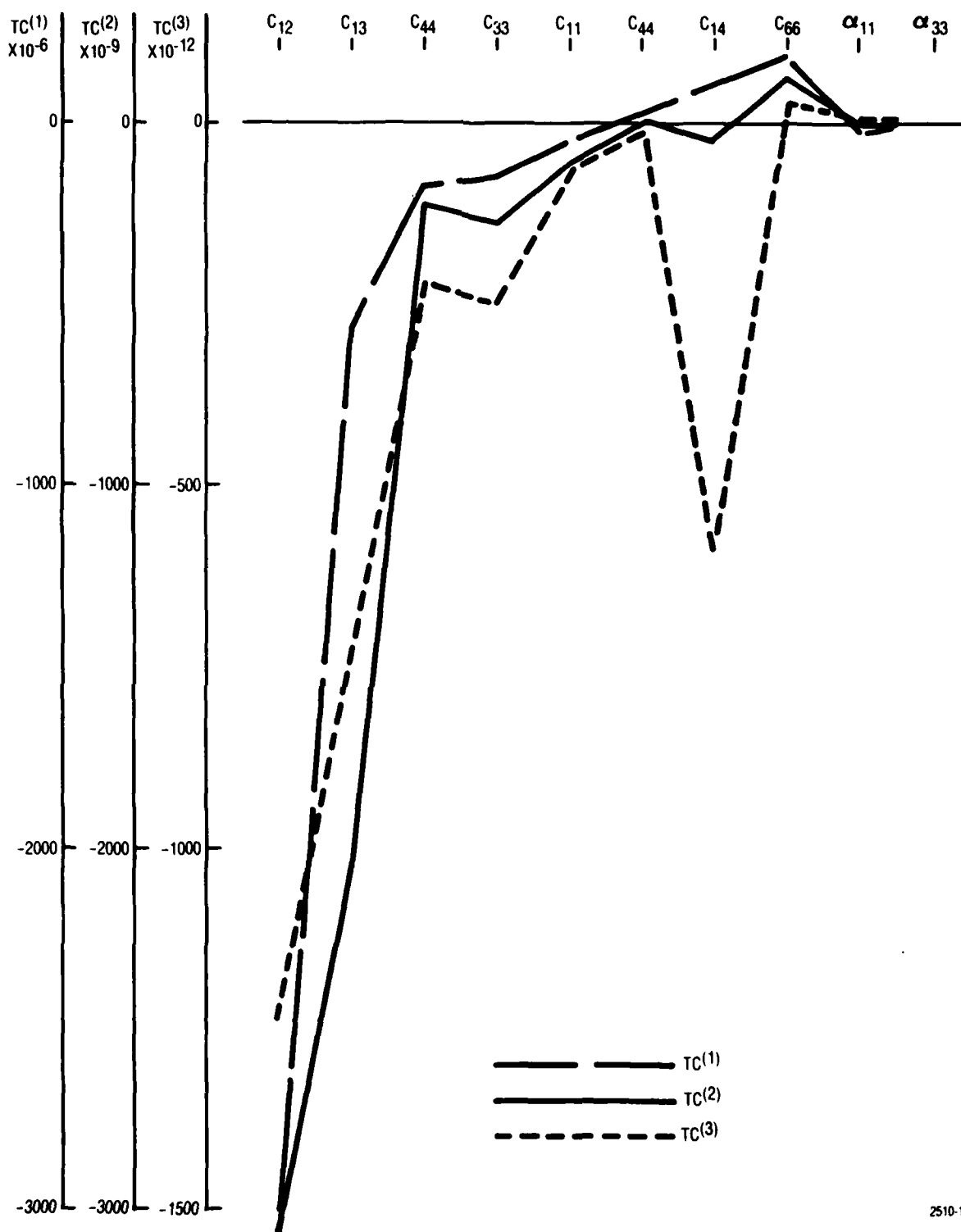


Figure 6. Temperature Coefficients of the Fundamental Constants of Quartz

Thus the most significant term is the first order term. The second order term is still quite significant but one order of magnitude below the first, while the third order term is almost three orders of magnitude below the first. Since the delay time τ is dependent on the crystal constants, the most significant term should be $TCF^{(1)}$. The least significant term should be $TCF^{(3)}$. After numerous calculations of the TCFs for many orientations, this appears to be the case.

The investigative approach used has been to first locate the surfaces of zero $TCF^{(1)}$ (the most significant term) with the finite difference program. Near these surfaces of zero $TCF^{(1)}$, low values of $TCF^{(2)}$ are sought, using already calculated results of the finite difference programs. Where low values of $TCF^{(2)}$ have been found, the perturbation approach was used to more accurately locate the zero $TCF^{(1)}$ surface, this being the most significant term in the total temperature dependence. $TCF^{(3)}$'s are then calculated to assure that their effect on the total temperature dependence is small. To date, this has always been found to be the case.

(8) Results of the Investigative Approach

Table 2 consists of a summary of the results of using the investigative approach described in paragraph (7) above. There are three areas where low TCF cuts have been located. These areas are centered near (YX wlt) 0/27/138, (YX wlt) 7/27/135.5, and (YX wlt) 15/40/40. These orientations have zero $TCF^{(1)}$, calculated by the Sinha and Tiersten approach, with $TCF^{(2)}$ and $TCF^{(3)}$ calculated with Finite Difference approach. These areas were chosen because of zero $TCF^{(1)}$, low $TCF^{(2)}$, and a low $TCF^{(3)}$ which can be mostly cancelled out by the first order TCF if the propagation direction is slightly rotated away from the zero $TCF^{(1)}$ direction. Then the $TCF^{(2)}$ term will dominate the performance characteristics. The angular resolution in these areas is $1^\circ \times 1^\circ \times 1^\circ$. The cuts potentially have one half to one third the temperature coefficients of ST-Cut quartz.

TABLE 2. PROPAGATION CHARACTERISTICS OF SELECTED ORIENTATIONS

Angles of ZTCF ⁽¹⁾ , Degrees (S & T's Program)			TCF ⁽²⁾ /°C ² (x10 ⁻⁸) Finite Difference Program	TCF ⁽³⁾ /°C ³ (x10 ⁻¹⁰) Finite Difference Program
Phi	Theta	Psi		
6	26	136.31	-1.4	
6	27	135.93	-1.3	0.67
6	28	135.59	-1.3	0.57
7	26	135.99	-1.5	
7	27	135.64	-1.4	
7	28	135.27	-1.3	0.65
8	26	135.74	-1.4	0.65
8	27	135.36	-1.4	
8	28	134.97	-1.3	
1	26	137.78	-1.2	0.68
1	27	137.48	-1.2	0.65
1	28	137.17	-1.1	0.67
0	26	138.07	-1.2	0.67
0	27	137.78	-1.1	0.68
0	28	137.49	-1.1	0.62
-1	26	138.37	-1.2	0.60
-1	27	138.09	-1.2	0.62
-1	28	137.80	-1.1	0.73
14	39	40.195	-1.0	0.64
14	40	40.415	-1.0	0.66
14	41	40.64	-1.0	0.75
15	39	39.79	-1.0	0.63
15	40	40	-1.0	0.74
15	41	40.23	-1.0	0.73
16	39	39.4	-1.0	0.68
16	40	39.605	-1.0	0.66
16	41	39.825	-1.1	0.60

d. Piezoelectric Coupling Factor

The piezoelectric coupling factor, denoted by k^2 , is a measure of the coupling efficiency for an interdigitated electrode.

We can express k^2 in terms of the interdigital transducer's input conductance¹ as

$$G_{in}(\omega_n) = -\pi^2 \omega_n M^2 W \epsilon_s^{(\infty)2} G_s P_{n-1}^2 (\cos \eta \pi) / K^2 (\cos \eta \pi / 2) \quad (18)$$

where $\omega_n = 2\pi(2n-1)/\lambda s_n$, M is the number of electrode pairs, w is the length of the electrodes, λ is the spatial periodicity of the array, the width of each electrode is $\eta\lambda/2$, $\epsilon_s^{(\infty)}$ is the value of the effective permittivity at zero velocity, K is the complete elliptic integral of the first kind, and P_n are the Legendre polynomials. G_s is the residue of $1/(s|\epsilon_s)$.

k^2 is defined by

$$k^2 = -2\epsilon_s^{(\infty)} G_s \quad (19)$$

Thus (18) becomes

$$G_{in}(\omega_n) = (1/2) \pi^2 \omega_n M^2 W \epsilon_s^{(\infty)} k^2 P_{n-1}^2 (\cos \eta \pi) / K^2 (\cos \eta \pi / 2) \quad (20)$$

and we see that k^2 is related to the input conductance and hence to the coupling efficiency. A good approximation to k^2 is given by

$$k^2 \cong 2(V_o - V_s)/V_s = 2\Delta V/V \quad (21)$$

where V_s is the shorted Rayleigh wave velocity and V_o is the free Rayleigh wave velocity.

It is seen that the quantity $\Delta V/V$ is an important parameter as it is a direct measure of the coupling efficiency and conductance of an interdigitated electrode pair on a piezoelectric substrate. Furthermore, $\Delta V/V$ is easily determined once the shorted and free surface problems have been solved. Programs are available for calculating the Rayleigh wave velocity with either shorted or free boundary conditions.

The shorted velocity calculations assumes a massless, perfectly conducting layer on the surface of the crystal. The boundary condition which must be satisfied is that $\phi = 0$ at $x_3 = 0$. The free surface boundary conditions are such that the potential ϕ and the normal component of the displacement, D_3 , are continuous at the surface. Furthermore, ϕ must satisfy Laplace's equation above the surface, resulting in

$$\phi = \phi_o \exp(-kx_3) \exp(-ik(x_1 - Vt)), \quad (x_3 \geq 0) \quad (22)$$

¹"Surface Wave Filters," Matthews, Herbert, John Wiley & Sons, New York (1977).

In both calculations the mechanical boundary conditions are the same, that there be no force component in the x_1 direction, or

$$T_{11} = T_{12} = T_{13} = 0 \text{ at } x_1 = 0 \quad (23)$$

$\Delta V/V$ for different crystal types with various orientations were calculated. Results have been found to be in good agreement with experiments.

For example, on ST-quartz,

$$\begin{aligned} V_o &= 3.1586 \times 10^3 \text{ m/s} \\ V_s &= 3.1569 \times 10^3 \text{ m/s} \\ \Delta V/V &= 5.4 \times 10^{-4} \end{aligned} \quad (24)$$

To insure the suitability of the cuts described in paragraph (8) above for SAW applications, the coupling coefficients have been calculated for these cuts and are summarized in Table 3.

TABLE 3. PROPAGATION CHARACTERISTICS OF SELECTED ORIENTATIONS

Angles of ZTCF ⁽¹⁾ , degrees (S & T's program)			Velocity (msec)	K ² ($\times 10^{-3}$)	Power Flow Angle (Degrees)
Phi	Theta	Psi			
6	26	136.31	3296.84	1.12	-0.3
6	27	135.93	3293.60	1.12	-0.2
6	28	135.59	3290.63	1.12	-0.1
7	26	135.99	3303.33	1.12	-0.5
7	27	135.64	3299.70	1.12	-0.4
7	28	135.27	3296.33	1.12	-0.3
8	26	135.74	3310.15	1.12	-0.7
8	27	135.36	3306.11	1.12	-0.6
8	28	134.97	3302.32	1.10	-0.5
1	26	137.78	3268.80	1.10	+0.7
1	27	137.48	3267.44	1.10	+0.9
1	28	137.17	3266.36	1.10	+1.0
0	26	138.07	3264.09	1.12	+0.9
0	27	137.78	3263.09	1.10	+1.1
0	28	137.49	3262.35	1.10	+1.2
-1	26	138.37	3259.65	1.10	+1.1
-1	27	138.09	3259.01	1.10	-1.3
-1	28	137.80	3258.64	1.08	+1.5

TABLE 3. PROPAGATION CHARACTERISTICS OF SELECTED ORIENTATIONS (CONT)

Angles of ZTCF ⁽¹⁾ , degrees (S & T's program)			Velocity (msec)	K ₂ (x10 ⁻¹)	Power Flow Angle (Degrees)
Phi	Theta	Psi			
14	39	40.195	3298.60	0.96	-7.7
14	40	40.415	3306.67	0.96	-8.1
14	41	40.64	3315.19	0.94	-8.6
15	39	39.79	3301.82	0.96	-7.8
15	40	40.00	3310.14	0.94	-8.3
15	41	40.23	3319.09	0.98	-8.6
16	39	39.4	3305.38	0.96	-8.0
16	40	39.605	3314.03	0.98	-8.4
16	41	39.825	3323.15	0.92	-9.0

e. Power Flow Angle

The power flow angle for a particular direction of propagation is an important design parameter. While the phase fronts always remain parallel to the source transducer, the wave, as a whole, does not propagate perpendicular to the wave fronts (see Figure 7). This is a characteristic of anisotropic substrates where the phase velocity is asymmetric about the propagation direction; i.e., $V(\psi + \Delta\psi) \neq V(\psi - \Delta\psi)$. The major problem which arises is that the acoustic beam may steer off of the desired propagation track, missing the output transducer unless it is properly designed.

The power per unit width carried in a surface wave is found by integrating the mechanical and electrical Poynting vectors to obtain

$$P_i = -\frac{1}{2} \operatorname{Re} \left\{ \int_{-\infty}^0 T_{ij} \mu_j^* dx_3 - i\omega \int_{-\infty}^{\infty} \phi D_i dx_3 \right\}, i = 1, 2 \quad (25)$$

P_1 gives the power flow perpendicular to the wave front and P_2 gives the power flow parallel to the wave front. $P_1 = 0$ for the Rayleigh wave which is confined to the surface. The power flow angle may be defined as

$$\theta = \arctan(P_2/P_1) \cong P_2/P_1 \text{ for } P_2 \ll P_1 \quad (26)$$

The power flow angles are calculated using either the perturbation programs or the finite difference routine. Table 4 gives results of calculations for the ST-Cut quartz. Note that for $\psi = 0$, the power

flow angle is zero, within the single precision accuracy used, as a result of the crystal symmetry. Power flow angles as high as 20 degrees are not uncommon on quartz.

TABLE 4. POWER FLOW ANGLES ST-CUT

ψ	Transverse/Incident Power	Power Flow Angle θ
0°	6.159×10^{-3}	0
10°	6.145×10^{-2}	3.5 degrees
20°	9.502×10^{-2}	5.4 degrees

The beam steering angle will be calculated for the selected cut of quartz with TCF = 0. The analytical results will be compared with experimental measurements. Table 3 contains the results of calculations for the selected orientations described in paragraph (8) above.

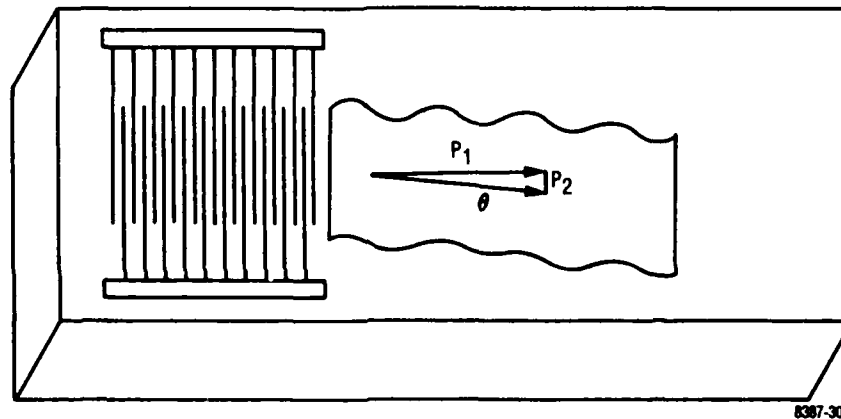


Figure 7. Nonzero Power Flow Angle

f. Proximity and Excitation Strength of Bulk Acoustic Waves (BAW) Spectrum

The purpose of this task is to analytically determine the strength of spurious signals caused by BAW. With this knowledge, one can predict the quality of the SAW device which has been selected for its zero TCD cut.

Interdigital transducers do not couple all of their field energy into surface waves. Bulk waves are also generated at various frequencies in the piezoelectric medium. These bulk waves can bounce off of the bottom surface, undergoing mode conversions in the process, and be received by the output transducer, resulting in unacceptable spurious signals. In most cases, this problem can be virtually eliminated by proper preparation of the bottom surface.

A transducer with periodicity λ excites surface waves at center frequencies

$$f_{SAW} = (2n + 1)V_{SAW}/\lambda \quad (27)$$

where V_{SAW} is the surface wave velocity and n is an integer, $n = 0, 1, 2, \dots$. The coupling to higher harmonics depends on transducer design. Bulk waves are radiated into the medium at an angle θ at a center fundamental frequency

$$f_b = V_b(\theta) / [\lambda \cos(\theta)] \quad (28)$$

where $V_b(\theta)$ is the velocity of the bulk wave in that particular direction. Equation 28 is a statement of the Bragg condition (see Figure 8). If the medium is isotropic for each mode, V_b is a constant. In the general case, V_b depends on the direction of propagation and hence on θ . To calculate $V_b(\theta)$, the matrix of elastic constants are rotated through the angle θ in the standard way. The quasi-longitudinal velocity and quasi-shear velocities are calculated as¹:

$$\begin{aligned} V_l &= \{[C_{11}(\theta) + e_{11}^2(\theta)/\epsilon_{11}(\theta)]/\rho\}^{1/2} \\ V_{SH} &= \{[C_{66}(\theta) + e_{16}^2(\theta)/\epsilon_{11}(\theta)]/\rho\}^{1/2} \\ V_{SV} &= \{[C_{55}(\theta) + e_{15}^2(\theta)/\epsilon_{11}(\theta)]/\rho\}^{1/2} \end{aligned} \quad (29)$$

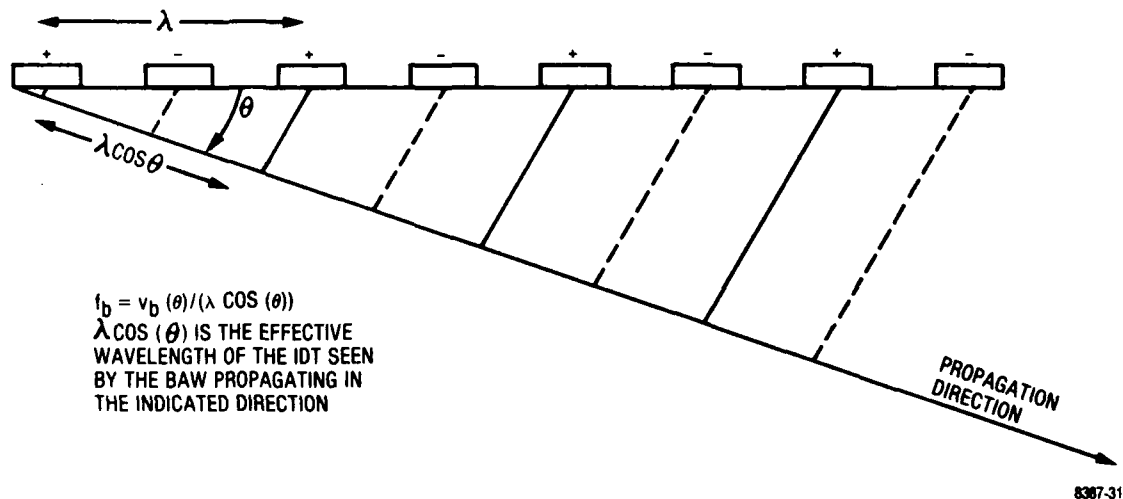


Figure 8. Bragg Condition for Excitation of BAW

The inverse values of these velocities, plotted as a function of θ , form the inverse velocity curves.

Inverse velocity plots as a function of propagation are particularly useful, for as long as $V_b/\cos \theta$, the effective velocity of the bulk wave on the surface, is greater than V_{SAW} , the effects of bulk mode generation may be suppressed by appropriate design and by proper conditioning of the bottom surface. Should $V_b/\cos \theta$ be less than V_{SAW} for any bulk mode, the SAW may couple to the BAW, resulting in a

¹"Physical Acoustics," Mason, Academic Press, NY, Vol. 1, Part A, 1964

leaky surface wave. Inverse velocity plots have been made for orientations with promising SAW temperature characteristics to check for the possibility of leaky surface waves and minimum values of f_s calculated and compared with f_{SAW} .

The polar plots of the inverse velocities for a (YX wlt) 0/27/137.8 and 7/27/135.59 are shown in Figure 9 and Figure 10, respectively. The values of $(1/v_{bulk})$ for the two shear modes and one longitudinal mode for different propagation directions (θ) into the crystal are also shown in Figures 9 and 10. The inverse surface wave velocity for 0/27/137.8 is 3.06×10^{-4} , that for 7/27/137.8 is 3.03×10^{-4} . These values are larger than the maximum $(1/v_{bulk}) \cos \theta$ ($< 2.9 \times 10^{-4}$), therefore, the analysis indicates that a leaky mode does not exist (see Table 3 for the SAW velocities).

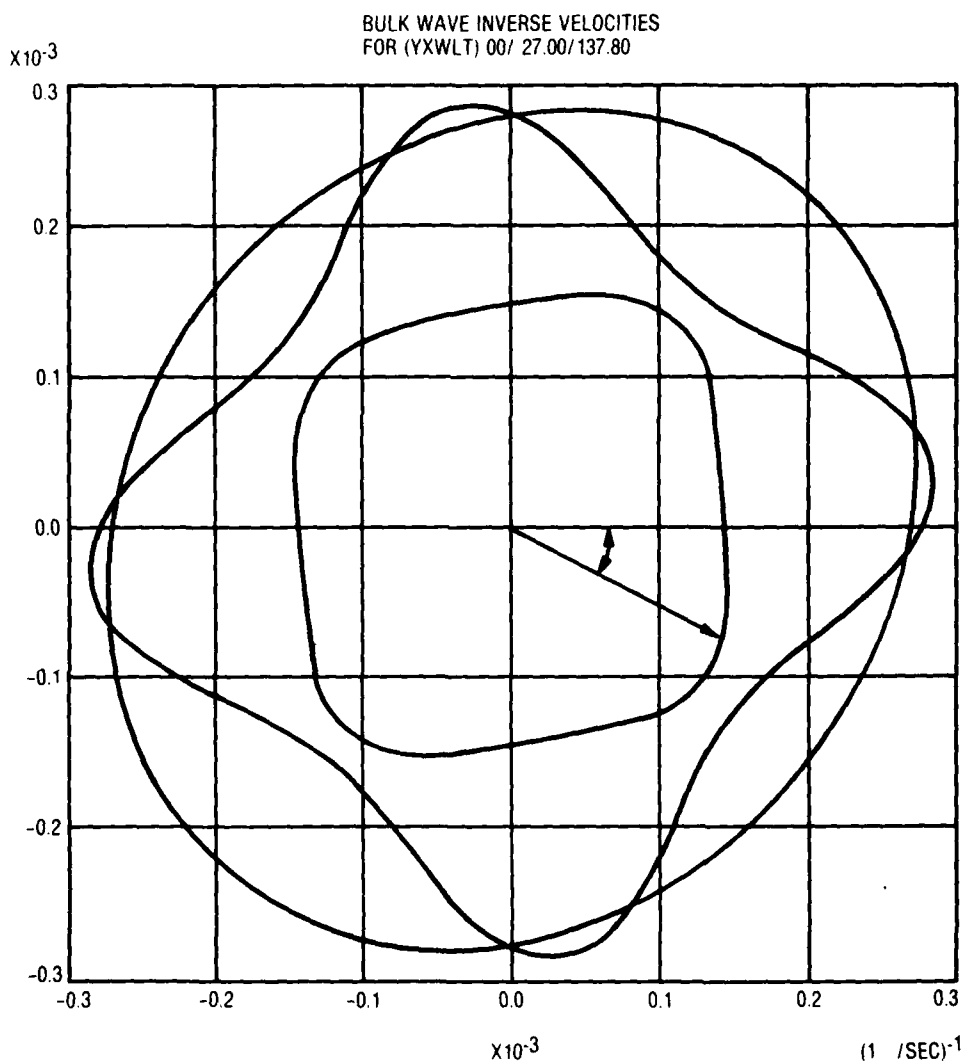


Figure 9. Polar Plots of Inverse Velocities for a (YXwlt) 0/27/137.8

2510-2

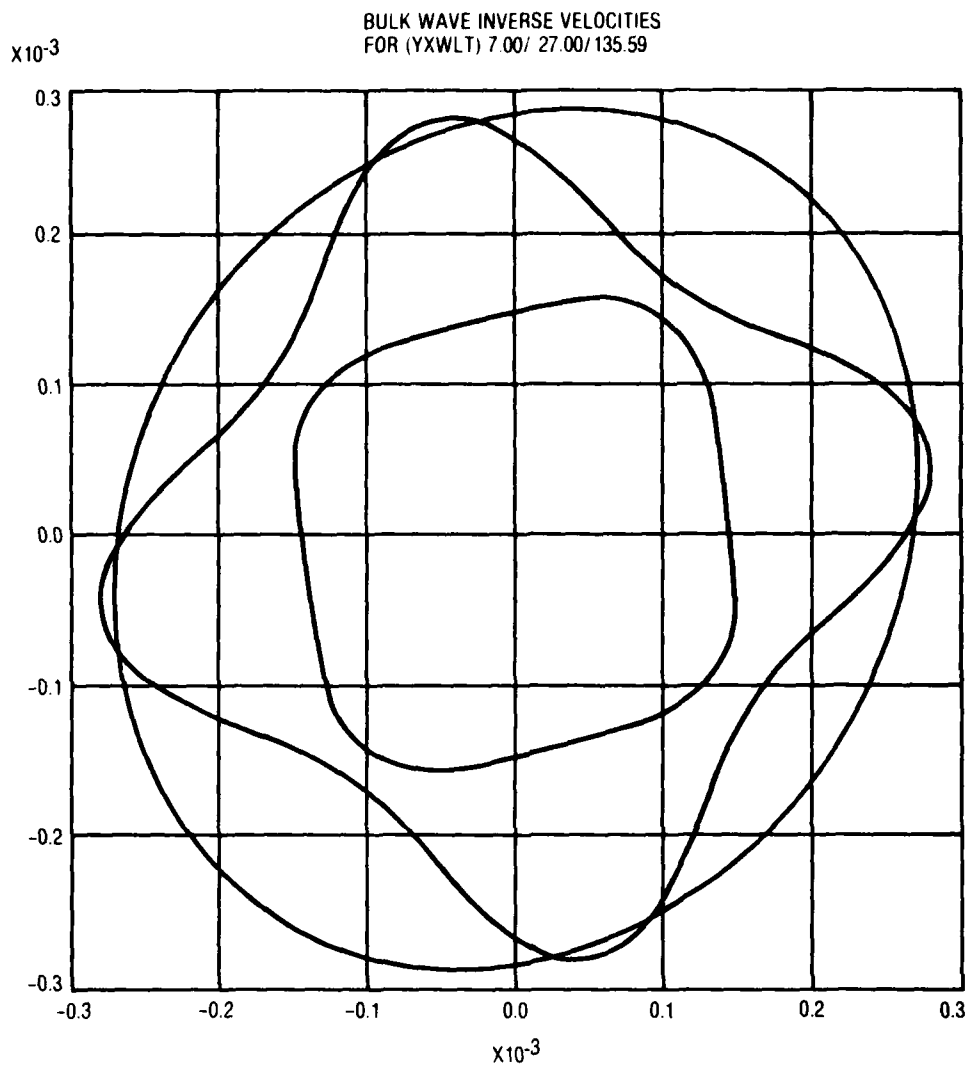


Figure 10. Polar Plots of Inverse Velocities for a (YXwlt) 7/27/135.59

2510-3

g. Degeneracies

Degenerate waves occur when the physical constants are such that equations (30) and (32) decouple.

$$\begin{bmatrix} \Gamma_{11} - \rho V_s^2 & \Gamma_{12} & \Gamma_{13} & \Gamma_{14} \\ \Gamma_{12} & \Gamma_{22} - \rho V_s^2 & \Gamma_{23} & \Gamma_{24} \\ \Gamma_{13} & \Gamma_{23} & \Gamma_{33} - \rho V_s^2 & \Gamma_{34} \\ \Gamma_{14} & \Gamma_{24} & \Gamma_{34} & \Gamma_{44} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} = 0 \quad (30)$$

where

$$\begin{aligned}
 \Gamma_{11} &= c_{55} b^2 + 2c_{15} b + c_{11} \\
 \Gamma_{22} &= c_{44} b^2 + 2c_{46} b + c_{66} \\
 \Gamma_{33} &= c_{33} b^2 + 2c_{35} b + c_{55} \\
 \Gamma_{12} &= c_{45} b^2 + (c_{14} + c_{56}) b + c_{16} \\
 \Gamma_{13} &= c_{35} b^2 + (c_{13} + c_{55}) b + c_{15} \\
 \Gamma_{23} &= c_{34} b^2 + (c_{36} + c_{45}) b + c_{56} \\
 \Gamma_{44} &= -(e_{33} b^2 + 2e_{13} b + e_{11}) \\
 \Gamma_{14} &= e_{35} b^2 + (e_{15} + e_{31}) b + e_{11} \\
 \Gamma_{24} &= e_{34} b^2 + (e_{14} + e_{36}) b + e_{16} \\
 \Gamma_{34} &= e_{33} b^2 + (e_{13} + e_{35}) b + e_{15}
 \end{aligned} \tag{31}$$

The boundary conditions become, in matrix form,

$$\begin{bmatrix}
 \dots (c_{3311} + c_{3313} b^{(m)}) \alpha_i^{(m)} + (e_{133} + e_{333} b^{(m)}) \alpha_4^{(m)} \dots \\
 \dots (c_{3111} + c_{3113} b^{(m)}) \alpha_i^{(m)} + (e_{131} + e_{331} b^{(m)}) \alpha_4^{(m)} \dots \\
 \dots (c_{3211} + c_{3213} b^{(m)}) \alpha_i^{(m)} + (e_{132} + e_{332} b^{(m)}) \alpha_4^{(m)} \dots \\
 \dots (e_{311} + e_{313} b^{(m)}) \alpha_i^{(m)} - (e_{31} + e_{33} b^{(m)} - i\epsilon_0) \alpha_4^{(m)} \dots
 \end{bmatrix}^T \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{bmatrix} = 0 \tag{32}$$

The definition of the constants and derivation of the equations are given in Appendix C. The condition for decoupling requires that the matrix in equation 30 has zero elements such that independent, non-Rayleigh wave solutions may exist. Equation 30 may decouple in many ways. If, for example, $\Gamma_{12} = \Gamma_{14} = \Gamma_{34} = 0$, u_1 and u_3 are found to be coupled and u_2 and ϕ are found to be coupled, however u_1 and u_3 are decoupled from u_2 and ϕ . If the physical constants are such that these two solutions are not coupled through the boundary conditions (equation 32) then we find the Rayleigh like wave (u_1 and u_3) is not coupled to ϕ , the potential term, and cannot be excited by electrodes in this cut.

The displacement u_2 which is coupled to ϕ is called the Bleustein — Gulyaev wave and is excited by interdigital transducers. These two waves (u_3 , u_1 and u_2 , ϕ) are degenerate as they propagate with the same velocity. The simplest method to determine whether equation 30 has decoupled for a particular orientation is to calculate the matrix of equation 30. This is presently accomplished using the Rayleigh wave velocity calculation program, which calculates and prints the matrix in equation 30. Because of the variety of special cases¹ which may arise, some of which may ultimately prove useful, each case in which we find the wave equation decouples will be considered on an individual basis.

¹"Propagation of Piezoelectric Surface Waves on Cubic and Hexagonal Crystals," Cambell & Jones, J.A.P., Vol. 41:2796-2801 (1970).

The analytical results of this section allow us to determine which modes can be generated on the selected zero TCD cut of quartz. At the three areas tabulated in Table 2, only Rayleigh wave modes were found.

h. Sensitivities Due to Crystal Misorientation

In cutting quartz and aligning masks on it, there is always some maximum achievable accuracy. Thus it is useful to know how all of the acoustic quantities considered vary with angle. Quantities such as TCD, phase velocity, power flow angle, $\Delta V/V$, bulk wave spectrums, and bulk wave velocity surfaces, are of interest to this program. These quantities can be accurately determined by directly calculating the quantities at $\phi = (\phi_0 + \Delta\phi)$, $\theta = (\theta_0 + \Delta\theta)$, and $\psi = (\psi_0 + \Delta\psi)$ with the same computer program discussed in paragraph 1, where ϕ_0 , θ_0 and ψ_0 are the desired angles, $\Delta\phi$, $\Delta\theta$ and $\Delta\psi$ are the actual directional deviation from the desired direction due to the fabrication tolerance. It is important to calculate the sensitivity of the parameters to the crystal misorientation; i.e., amount of change of a function as a result of small angular misorientation.

For case of the power flow angle (PFA)

$$\begin{aligned} d[\text{PFA}(\phi = 0, \theta = 42.75, \psi = 10^\circ)]/d\psi \\ \cong (\text{PFA}(\psi = 20^\circ) - \text{PFA}(\psi = 0^\circ))/20^\circ \\ \cong 0.27^\circ/\text{degree}. \end{aligned} \quad (33)$$

The quantities $d[\text{PFA}(\phi = 0^\circ, \theta = 42.75, \psi = 10^\circ)]/d\phi$ and $d[\text{PFA}(\phi = 0^\circ, \theta = 42.75^\circ, \psi = 10^\circ)]/d\theta$ are computed in an equivalent manner.

In the case of TCD:

$$d(\text{TCD}) = \frac{\partial(\text{TCD})}{\partial\theta} d\theta + \frac{\partial(\text{TCD})}{\partial\phi} d\phi + \frac{\partial(\text{TCD})}{\partial\psi} d\psi \quad (34)$$

$$\frac{\partial(\text{TCD})}{\partial\theta} = [\text{TCD}(\phi_0, \theta_0, \psi_0) - \text{TCD}(\phi_0, \theta_0 + \Delta\theta, \psi_0)]/\Delta\theta \quad (35)$$

$$\frac{\partial(\text{TCD})}{\partial\phi} = [\text{TCD}(\phi_0, \theta_0, \psi_0) - \text{TCD}(\phi_0 + \Delta\phi, \theta_0, \psi_0)]/\Delta\phi$$

$$\frac{\partial(\text{TCD})}{\partial\psi} = [\text{TCD}(\phi_0, \theta_0, \psi_0) - \text{TCD}(\phi_0, \theta_0, \psi_0 + \Delta\psi)]/\Delta\psi$$

All the TCD (ϕ, θ, ψ) and TCD ($\phi, \theta, \psi + \Delta\psi$) etc., are calculated with the computer programs discussed in paragraph 1. Therefore, all the $\partial(\text{TCD})/\partial\theta$, $\partial(\text{TCD})/\partial\psi$, $\partial(\text{TCD})/\partial\phi$ can be accurately calculated. Hence the sensitivities due to crystal misorientation are determined.

Calculation of the angular dependence on the first, second, and third order TCDs is, of course, our primary task. Of these three quantities, the first order TCF is most sensitive to angular variation. The

angular dependence on these parameters will be calculated in the same way as all of the other quantities but on a much smaller angular grid ($\Delta\theta$, $\Delta\phi$ and $\Delta\psi$) about the zero TCD locus. The size of this grid will vary, depending on the magnitude and smoothness of the variation about each point on the locus of zero first order TCD orientations as verified by experiment and calculation. In case the function is smooth or linearly varying with angles, large Δ angles may be used.

By performing the above mentioned calculations, we have precise information on the sensitivities due to crystal misorientation. This information will allow us to impose a practical tolerance limit on fabrication and still be able to achieve the required superior performance specification.

Quantities such as velocity (Table 3), power flow angles (Table 3), BAW spectrum (Figures 50 and 51), coupling coefficients (Table 3), and second and third order TCFs (Table 2) do not vary quickly with angle. This is not the case for $TCF^{(1)}$. Table 5 contains a summary of $\partial TCF^{(1)}/\partial\psi$. The large values of $\partial TCF^{(1)}/\partial\psi$ impose strict fabrication tolerances on the SAW cuts and mask alignment. Fabrication accuracy to within 6 minutes is required to keep the total temperature variation due to $TCF^{(1)}$ within 45 ppm for $\partial TCF^{(1)}/\partial\psi = 3(\text{PPM}/^{\circ}\text{C})/\text{degree}$ over the temperature range -50°C to 100°C . Table 6 contains summaries of $\partial TCF^{(1)}/\partial\phi$ and $\partial TCF^{(1)}/\partial\theta$. These values impose fabrication tolerances on the rotated quartz plate angles ϕ and θ of 12 minutes to keep the total temperature variation due to $\partial TCF^{(1)}(15/40/40)/\partial\phi$ within 45 ppm over the temperature range -50°C to 100°C . This linear temperature variation may be compensated for by varying ψ on any particular cut if all other cut parameters vary slowly with angle.

TABLE 5. $\partial TCF^{(1)}/\partial\psi$ FOR SELECTED CUTS

Angles of ZTCF ⁽¹⁾ , degrees (S & T's program)			$\partial TCF^{(1)}/\partial\psi$
Phi	Theta	Psi	
6	26	136.31	+2.7 (ppm/C°)/degree
6	27	135.93	+2.7
6	28	135.59	+2.7
7	26	135.99	+2.7
7	27	135.64	+2.7
7	28	135.27	+2.7
8	26	135.74	+2.7
8	27	135.36	+2.7
8	28	134.97	+2.7
1	26	137.78	+2.8

TABLE 5. $\partial TCF^{(1)}/\partial \psi$ FOR SELECTED CUTS (CONT)

Angles of ZTCF ⁽¹⁾ , degrees (S & T's program)			$\partial TCF^{(1)}/\partial \psi$
Phi	Theta	Psi	
1	27	137.48	+2.8
1	28	137.17	+2.8
0	26	138.07	+3.0
0	27	137.78	+3.0
0	28	137.49	+3.0
-1	26	138.37	+3.0
-1	27	138.09	+3.0
-1	28	137.80	+3.0
14	39	40.195	-3.5
14	40	40.415	-3.5
14	41	40.64	-3.5
15	39	39.79	-3.5
15	40	40	-3.5
15	41	40.23	-3.5
16	39	39.4	-3.7
16	40	39.605	-3.7
16	41	39.825	-3.7

TABLE 6. $\partial TCF^{(1)}/\partial \phi$ AND $\partial TCF^{(1)}/\partial \theta$ FOR SELECTED CUTS

Angles of ZTCF ⁽¹⁾ (S&T's Program), Degrees			$\partial TCF^{(1)}/\partial \phi$	$\partial TCF^{(1)}/\partial \theta$
Phi	Theta	Psi		
7	27	135.64	-0.7(ppm/C°)/degree	-0.5(ppm/C°)/degree
0	27	137.78	-0.8	-0.8
15	40	40.00	+1.5	-0.7

2. WAFER FABRICATION

During the developmental phase of the doubly rotated cut SAW Devices program, a large number of wafers with 30 different crystal orientations will be fabricated and evaluated. To perform this task with good quality control, minimum cost and in a short time, Motorola has developed the techniques and processes to fabricate the doubly rotated cut of quartz wafers internally. The crystal boules are supplied by Motorola.

Carlisle, Pennsylvania; the X-ray wafer cutting is performed at Motorola's Semiconductor Group; polishing, fabrication and testing are performed at the Motorola Government Electronics Division. The methods used to fabricate the quartz wafers are described in the following sections.

A computer program was developed to calculate the incident angles and reflected angles for any given cut of crystal. The basic mathematical relations were derived in R.A. Heising's "Quartz Crystals for Electrical Circuits." The relations were formulated to computer programs. The flow diagram is shown in Figure 11. The results are shown in the printout (see Appendix F). The incident angle G , exit angle $(G + G')$, are defined for each plate position. The plate positions are determined by the direction of the rotated axis, $(\pm 1, \pm 2, \pm 3)$, relative to the measuring stage. Once the angles of $(YX \text{ wlt}) \phi/\theta/\psi$ are defined, all of the reflection angles will be calculated for the different reflection planes, defined by Miller indicies. The useful reflection planes that provide intense reflection with low skewed angles (< 5 degrees) are selected for printout. These results, after modification due to change in standards, are used to check the accuracy of the cuts.

a. Face Definitions

The following is an outline of the procedure to be used in this program to make a doubly rotated cut $(YX \text{ wlt}) \phi/\theta/0$. The quartz bars have four lumbered faces with the minus X axis marked. The opposite face is marked by coloring it with a magic marker (blue). One other face not opposite the $-X$ face is colored also with a magic marker (red). The red face is now defined to be the $+Z$ axis as in Figure 12. The direction of the $+Y$ axis may be found by using the right-hand rule ($+X$ crossed into $+Y$ gives $+Z$). The $+Y$ axis will lie along the length of the crystal. Note that there are two ways to set up the axes on the crystal corresponding to choice of the red face (see Figure 12).

b. Running the X-Ray Program

The X-ray orientation program XRAY is run with the angles $\phi/\theta/0$. The sequence of instructions on the Honeywell 560 under the CP-V operating system is as follows:

!SET F:103 DC/MILDAT .538; IN

(This instruction assigns to unit 103 the file containing all of the Miller indicies to be searched.)

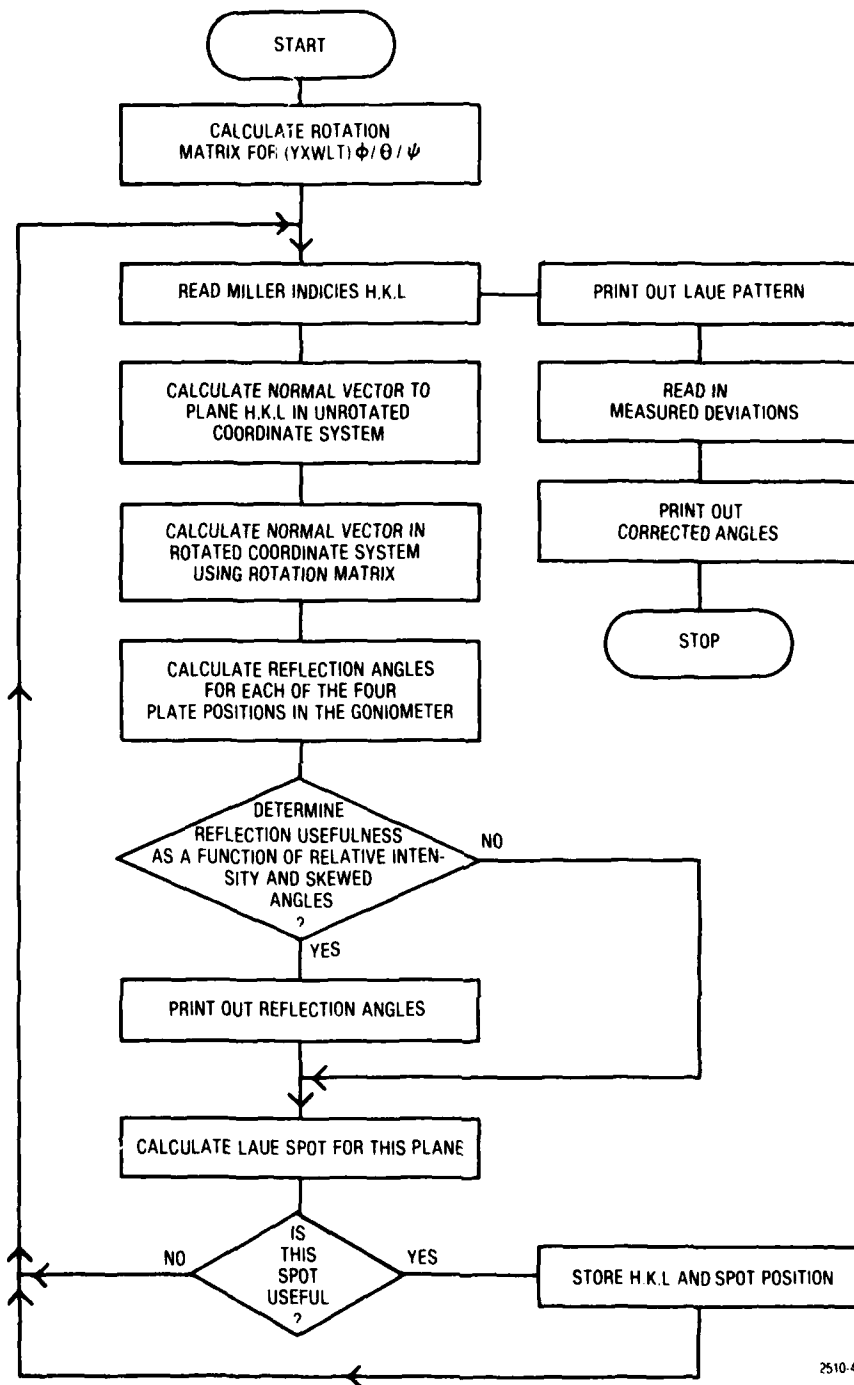
!SET F:104 DC/ERRDAT .538; IN

(This instruction assigns to unit 104 the file containing all of the angle perturbations defined in Heising for use with the Laue photographs.)

!XRAYL M.538

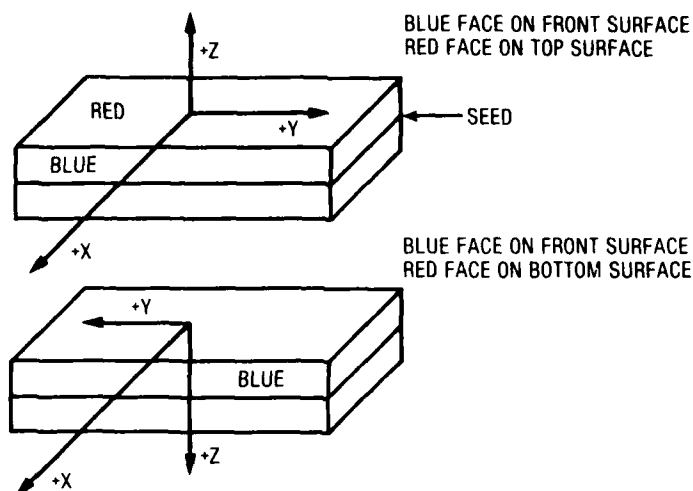
(This instruction loads and begins execution of the program.)

The program will ask for the angles $\phi/\theta/0$. These angles are entered in 3G format [i.e., 10.0, 3.0, 0.0 (carriage return)] and the results of the X-ray analysis printed.



2510-4

Figure 11. Flow Diagram of Calculation for Reflected Angles in Doubly Rotated Cut of Quartz



. 510-5

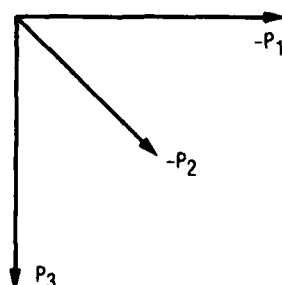
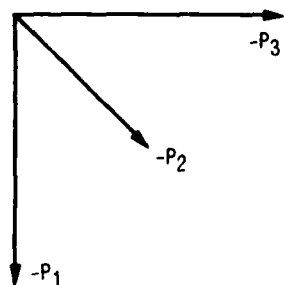
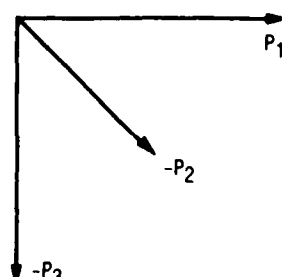
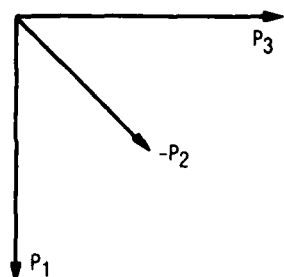
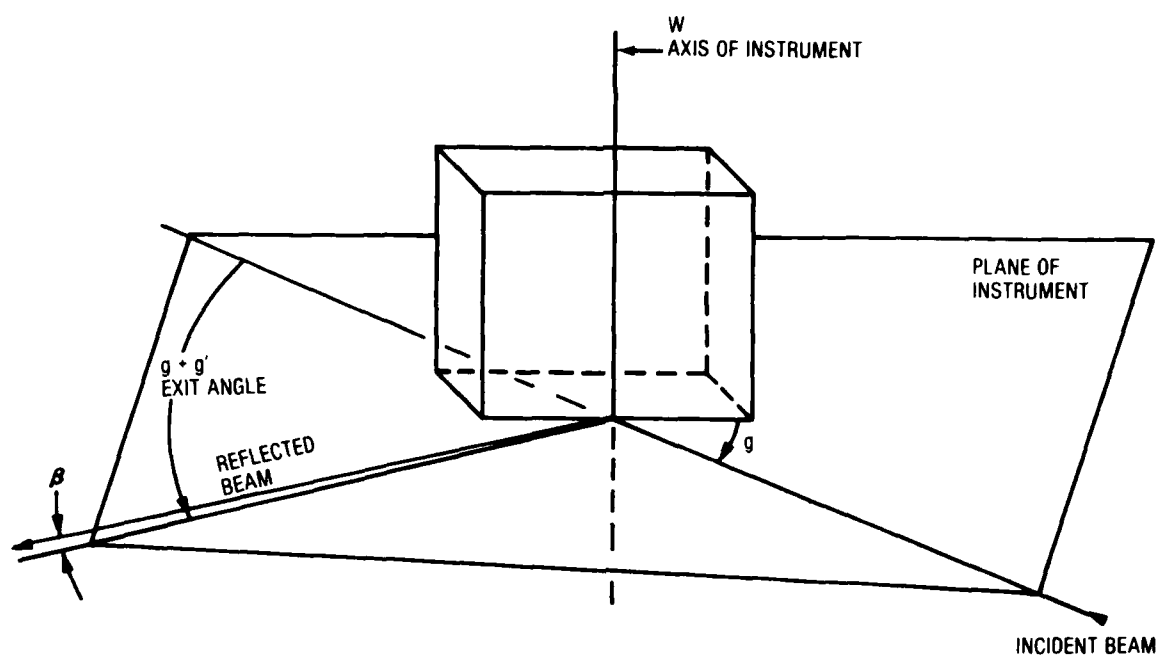
Figure 12. Two Possible Ways of Defining the Crystal Axes on a Lumbered Bar

c. Analysis of X-Ray Program

The X-ray program used follows the development of Heising's which uses a book written before the 1949 IRE Standard we use now. His X, Y, and Z axes will be denoted as $\bar{X}$, $\bar{Y}$, and $\bar{Z}$. The relation to our standard is as follows:

Heising	1949 IRE Standard
$+\bar{X}$	$-X$
$+\bar{Y}$	$-Y$
$+\bar{Z}$	$+Z$

Furthermore, Heising's incident beam comes from the left, while our incident beam comes from the right. When these differences are accounted for, the "position chart" shown in Figure 13 must be used instead of the charts Heising uses in order that our X-ray machine and the 1949 standard may be used. P_1 , P_2 , and P_3 in the "position chart" are the $+X$, $+Y$, and $+Z$ axes of the rotated plate. An important note of caution: the ϕ crystal face off of which we reflect the X-ray beam has $\bar{Y}$ or $-Y$ as its normal. Since we may not assume that the crystal faces are parallel, we must propagate the surface wave on this face. This is important, because to achieve the same crystal properties, we must rotate by ψ about the $+Y$ axis, resulting in a change of the sign of the third rotation (see Figure 14).



POSITION 1

POSITION 2

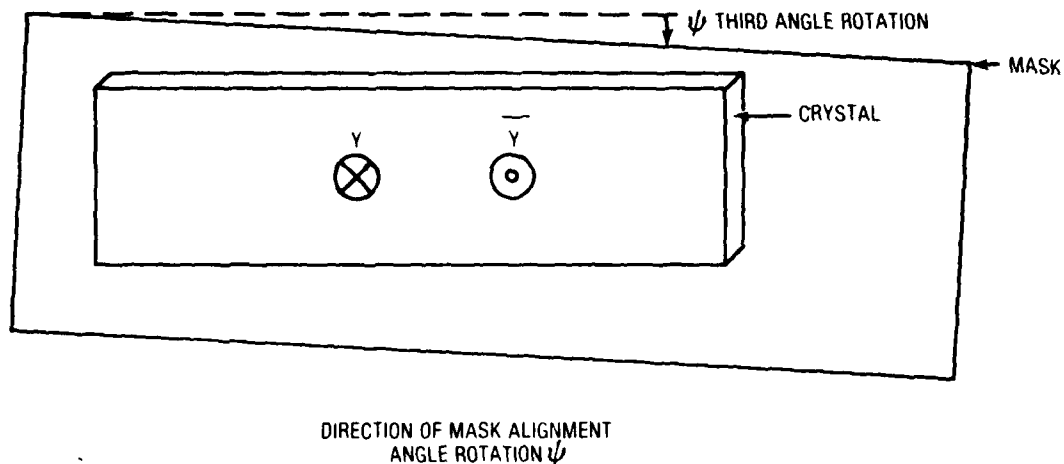
POSITION 3

POSITION 4

2510-7

P_1 , P_2 , and P_3 are the rotated plate axes X, Y, and Z.

Figure 13. X-ray Position Chart



2510-6

Figure 14. Direction of Mask Alignment Angle Rotation ψ

d. Determination of the Actual ψ Angle

The third angle of rotation must be measured from a reference. The reference used is the face opposite the red face of the crystal ($-Z$ face). To determine the actual orientation of the finished crystal edge, we must know the orientation of this plane exactly (see Figure 15).

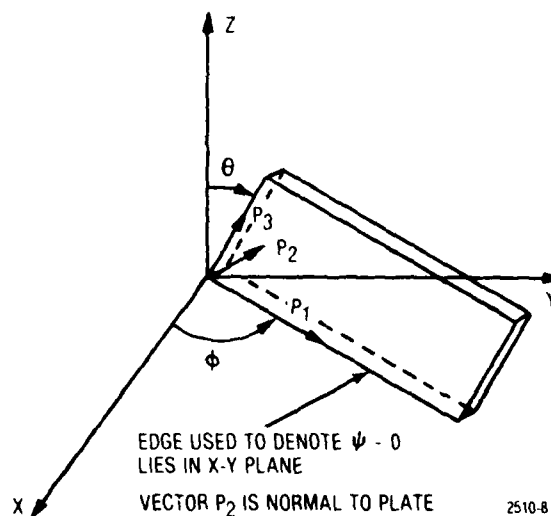


Figure 15. Crystal Rotation (YX wlt) $\phi/\theta/0$

If the angles α and β in Figure 16 are measured using the (003) plane, which is parallel to the X and Y axes, $\Delta\psi$ is given by:

$$\Delta\psi = -\tan^{-1} [(-\cos \phi \sin \alpha - \sin \phi \sin \beta) / (\sin \theta \sin \phi \sin \alpha - \sin \theta \cos \phi \sin \beta + \cos \theta \sqrt{1 - \sin^2 \alpha - \sin^2 \beta})] \quad (36)$$

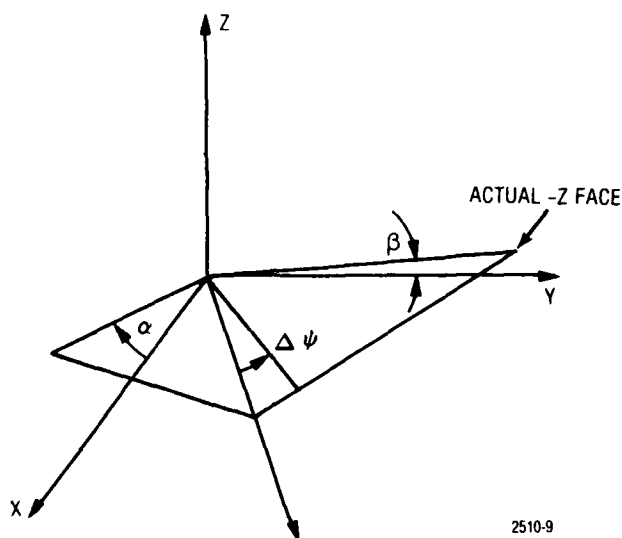


Figure 16. Actual -Z Face, Crystalline Axes, α , β , and $\Delta\psi$

Thus, given a ψ desired which we wish to obtain, we must actually rotate the mask by $\psi_{\text{actual}} = \psi_{\text{des}} - \Delta\psi$ as shown in Figure 17.

e. Determination of α and β

The most appropriate crystal plane to use for determining α and β is the 003 plane. This plane has all of its atoms lying in planes perpendicular to the Z axis, and for a perfect Z face the X-ray deflection angles will be:

G = Angle of incidence = 25 degrees 19 minutes

$G + G'$ = Exit angle = 50 degrees 38 minutes

For all positions on the X-ray machine with the +Z or -Z face being X-rayed. To determine α and β for the -Z face, we use the following relationships.

$$\alpha = 1/2 (G_{\cdot X \text{ TOWARD INCIDENT}} - G_{\cdot X \text{ TOWARD INCIDENT}}) \quad (37)$$

$$\beta = 1/2 (G_{\cdot Y \text{ TOWARD INCIDENT}} - G_{\cdot Y \text{ TOWARD INCIDENT}}) \quad (38)$$

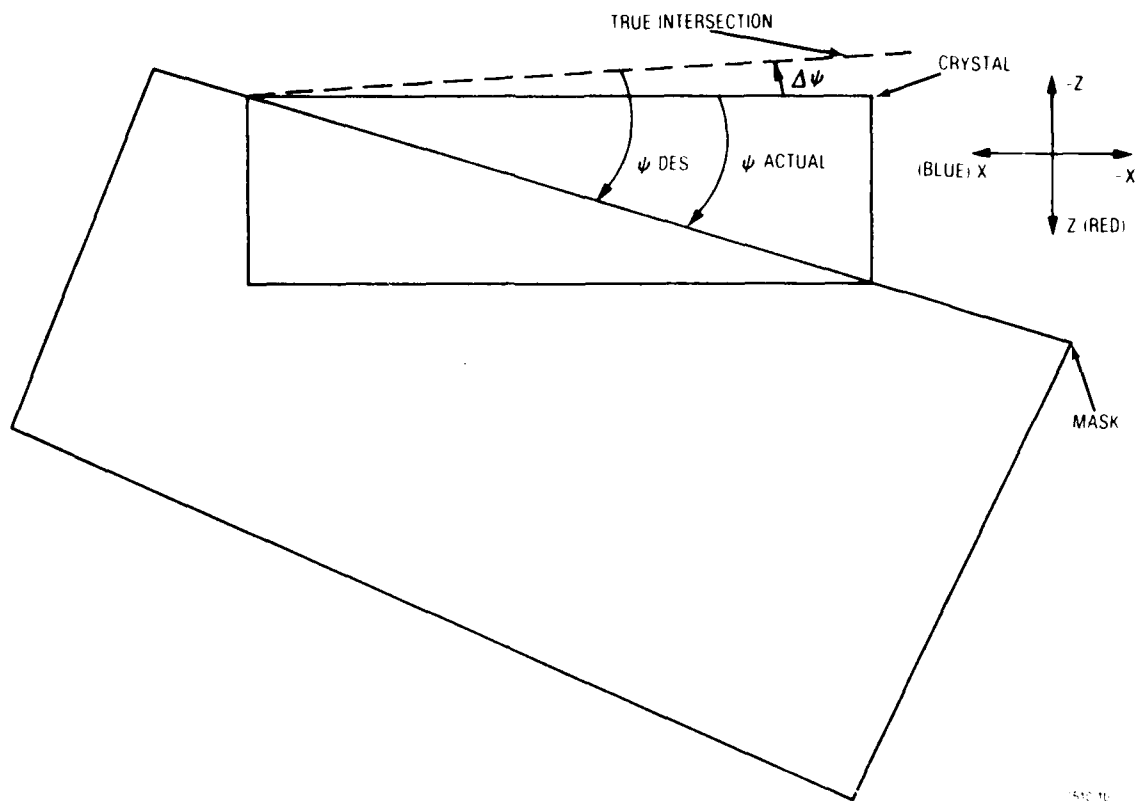


Figure 17. Mask Rotation to Obtain Desired ψ

To determine α and β for the +Z face we use

$$\alpha' = 1/2 (G_{-X} \text{ TO INCIDENT} - G_{-X} \text{ TO INCIDENT}) \quad (39)$$

$$\beta' = 1/2 (G_{-Y} \text{ TO INCIDENT} - G_{-Y} \text{ TO INCIDENT}) \quad (40)$$

α' and β' are the α and β we would have measured for a -Z face that is parallel to the +Z face measured, which means that equation (36) is still valid for α' and β' .

The quartz crystal will now have the orientation (YX wlt) $\phi/\theta/ - \Delta\psi(\alpha, \beta)$ if we use the -Z edge as a reference and (YX wlt) $\phi/\theta/ - \Delta\psi(\alpha', \beta')$ if we use the +Z edge as a reference. The computer X-ray program for these angular orientations must be used if we are to get an accurate measurement. The integrity of these measurements of α and β is checked by comparing $1/2 (G_{-X} + G_{+X})$ and $1/2 (G_{-Y} + G_{+Y})$ with the theoretical result, $G_{AVC} = 25$ degrees 19 minutes.

f. Procedure Used to Zero X-Ray Machine:

(1) Use reference quartz plate marked 10.1

- (2) Set X-ray exit angle to 26.5 degrees (marked AT cut on machine)
- (3) Set plate in X-ray machine with marking toward you (X-ray bounces off unmarked surface) and blue line up (width direction vertical). (See Figure 18).
- (4) Adjust with clutch till X-ray reading occurs at incident angle 13 degrees 18 minutes
- (5) Set plate in X-ray machine with marking toward you (X-ray bounces off unmarked surface) and blue line down (width direction vertical). (See Figure 19).
- (6) Angle of incidence should occur at 13 degrees 18 minutes + Δ angle.
- (7) Adjust clutch until angle of incidence is at 13 degrees 18 minutes + $1/2 \Delta$ angle.
- (8) Check alignment by measuring in positions of steps 3 and 5. The average of the two readings should be 13 degrees 18 minutes. Any discrepancy represents error in zeroing the machine and may be made less than less than 1 minute.
- (9) If the 10.1 cut is not available, the same procedure may be used if, for the cut to be used, the theoretical angles of incidence are equal for the particular crystal plane used in both positions.

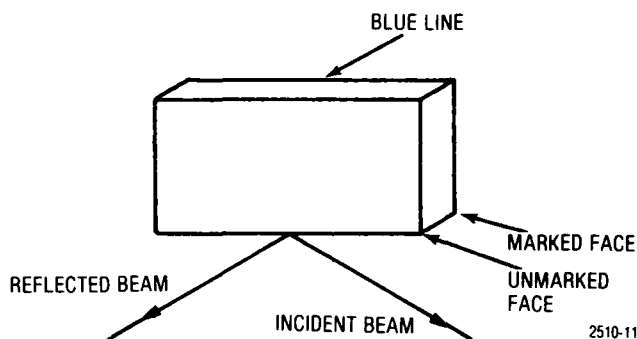


Figure 18. Position of Step 3, 10.1 Alignment Wafer

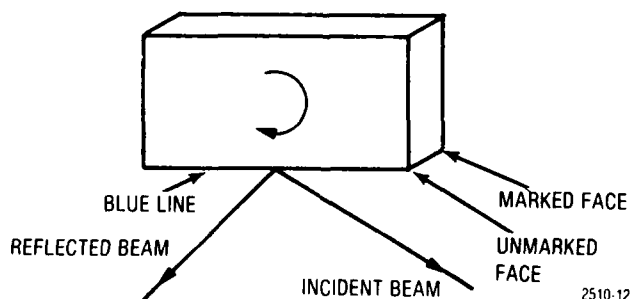


Figure 19. Position of Step 5, 10.1 Alignment Wafer Rotated by 180 Degrees About -Y Axis

g. Cutting Techniques for Doubly Rotated Orientations

A slicing machine built by Meyer and Burger Company, model TS3, was used to slice the quartz boule. The 6 inch diamond impregnated blade is supplied by Maurice Dessau, New York. The drift accuracy of the 2 inch cut is approximately 3 mils (~5 minutes).

The stage of the saw has the capability to rotate in two dimensions; it is designed to make the doubly rotated cut. The adjustment accuracies are graded to 0.5 minute. The X-ray beam resolution is about 2 minutes.

The combined accuracy of the wafers obtained experimentally has been better than 15 minutes. Iterative adjustment of the cutting stage can bring the cutting accuracy to within 10 minutes. The cutting procedures are the following:

- (1) Heat brass plate, glass plate and quartz boule.
- (2) Melt wax on brass plate and mount glass plate.
- (3) Melt wax on glass and mount quartz boule on glass.
- (4) Let cool to room temperature.
- (5) Screw mount brass plate to slice machine.
- (6) Initial cut of boule along the XZ plane (or directly to the desired angle if the boule was lumbered).
- (7) Determine true atomic plane using diffractometer and X-ray computer program.
- (8) Adjust stage to correct for true atomic planes, and obtain the desired rotation.
- (9) Perform doubly rotated cut of quartz.
- (10) Measure the reflection angle and check against the calculated result of the X-ray program. Iterative adjustment of stage can be done if cut accuracy is critical.

These procedures are presently used to cut the wafers with low TCF orientation required for this program.

h. Wafer Polishing

The polishing process for the quartz wafers was established during this period. The procedure includes the following:

- (1) The crystal axis orientation is marked on the back surface of the wafers with marking ink and baked dry. The markings have been demonstrated to stay on the crystal throughout the photolithographic process for easy identification.

(2) The corners of the wafers are ground prior to lapping and polishing to prevent corner breakage.

(3) The polishing is a two step process. The first step is a 15 μm lapping to obtain surface flatness with Microgrit, type WCA, Size 15, on a LAPMASTER, Model 24. The second step is to polish the surface with Cerium oxide on a LogiTech, Ltd. Model PM2 polisher. The polish wheel is made of pitch wax supplied by Hacker Instruments, Inc. The polished wafers have a surface finish with no observable grains or pits under a 50X microscope. The wafers are suitable for surface wave application. X-ray orientation was performed before and after the lapping and polishing processes. The change is normally less than 6 minutes. At the present time, wafers of the following cuts are polished; these are $\phi/\theta/\psi$ of 6/27/135.9, 6/28/135.6, 7/27/135.6, 7/28/135.3, 8/26/135.7, 8/27/135.4, and 8/28/134.9.

In the coming period, SAW devices will be fabricated on these wafers. Experimental results will be obtained and compared with the theoretical calculations.

SECTION III CONCLUSION

The temperature coefficients of frequency (TCF) have been analyzed for doubly rotated cuts of quartz for surface acoustic wave devices. The analysis procedure is shown below:

- (1) Using Finite Difference program, identify angular areas with zero $TCF^{(1)}$ and low $TCF^{(2)}$ on $10^\circ \times 10^\circ \times 10^\circ$ grid.
- (2) Calculate in these areas with $2.5^\circ \times 2.5^\circ \times 2.5^\circ$ grid to locate the rotation with minimum $TCF^{(2)}$ which has $TCF^{(1)} = 0$.
- (3) Identify the accurate zero $TCF^{(1)}$ with Sinha and Tiersten's program in areas obtained in (2).
- (4) Calculate $TCF^{(1)}$, $TCF^{(2)}$ and $TCF^{(3)}$ in selected areas obtained in (3) with $1^\circ \times 1^\circ \times 1^\circ$ span.
- (5) Calculate the coupling coefficients, propagation velocities, power flow angles and inverse bulk wave velocities for these angles.

The conclusions of the initial study are:

- (a) The zero $TCF^{(1)}$ surface and zero $TCF^{(2)}$ surface data does not show an intersection in the $10^\circ \times 10^\circ \times 10^\circ$ grid. However, orientations with frequency variation ≈ 100 ppm from -50°C to 100°C , *better than ST Cut by a factor of two*, have been found in several areas where $TCF^{(1)} = 0$ and $TCF^{(2)}$ is less than $1.5 \times 10^{-8}/^\circ\text{C}^2$.
- (b) The $\Delta TCF/\Delta$ angle is normally very large in the areas with zero $TCF^{(1)}$ and low $TCF^{(2)}$, therefore accurate crystal orientation is critical. It is estimated that the orientation accuracy of 6 minutes is required to obtain a $TCF^{(1)}$ of ≈ 50 ppm in the -50°C to 100°C temperature range in the three areas investigated. These are $\phi/\theta/\psi$ of 6/27/135.93 (4.45×10^{-2} ppm/ $^\circ\text{C} \cdot \text{minute}$), 14/40/40.415 (5.83×10^{-2} ppm/ $^\circ\text{C} \cdot \text{minute}$) and 0/27/137.78 (5.00×10^{-2} ppm/ $^\circ\text{C} \cdot \text{minute}$). Orientations with less sensitivity to orientation accuracy have been evaluated. These are the cuts that have $\partial[TCF^{(1)}]/\partial\psi = 0$ when $TCF^{(1)} = 0$. The cuts evaluated were $\phi/\theta/\psi = 20/30/155$, 20/20/150, 10/40/168. The $TCF^{(2)}$ of these cuts are approximately $4 \times 10^{-8}/^\circ\text{C}^2$, comparable or higher than ST cut.
- (c) Coupling coefficients, velocities and beam steering angles were defined for the selected areas, no leaky modes were found in these areas.
- (d) Methods to X-ray orient the quartz crystals, cut the doubly rotated wafers and polish such crystal wafers were developed. The wafers are ready for SAW device fabrication. The effort in the coming period is to design and fabricate single mode oscillators and to experimentally measure the TCF's of these selected orientations.

APPENDIX A

VOLUME PERTURBATION OF AULD

Perturbation techniques, as used here, allow calculations of small changes in the solutions to a problem caused by small changes in the physical parameters of the problem, once the solution to the unperturbed problem is known.

Our general approach to the problem of determining the temperature dependence of V_s will be as follows. First, the Rayleigh wave propagation problem will be solved in the standard way in its entirety at room temperature, T_0 . Given the solution of problem at T_0 and the dependence of the physical constants (such as c_{ij}) on temperature at T_0 , we will apply the volume perturbation formula, calculating the temperature dependence of V_s . The dependence of V_s on T is then used to calculate the frequency characteristics of the actual device given the thermal expansion coefficients as a function of temperature. At this point, the frequency temperature dependence of the substrate as a function of crystal cut and direction can be thoroughly explored.

The Volume Perturbed Formula.

Denoting $u_i(T_0)$ by u_i , etc., the volume perturbation formula is given by¹:

$$\beta_R = \omega \int_0^\infty [A] dy / \int_0^\infty (-u^* \cdot T' - u' \cdot T^* + \phi^* (i\omega D') + \phi' (i\omega D)^*) \cdot z dy \quad (A-1)$$

$$[A] = [\Delta \rho u^* \cdot u' + T^* : (\Delta s^E : T' + \Delta d \cdot E') + E^* \cdot (\Delta \epsilon^T \cdot E' + \Delta d : T')]$$

This equation is exact, but involves knowing the solution u' . However, we can set $u = u'$ if the temperature dependence of the solution is small and use $P = (1/2) \text{Re} \int (-u^* \cdot T + E \cdot H^*) dy$ to obtain the approximate solution

$$\Delta \beta_R = (\omega/4P) \int_0^\infty [\Delta \rho |u|^2 + S : \Delta c : S + E^* \cdot \Delta \epsilon^T \cdot E + E^* \cdot \Delta e : S + S : \Delta e \cdot E] dy \quad (A-2)$$

The u 's and E 's, and ρ come directly from the computer solution at T_0 .

¹Auld, B.A., "Acoustic Fields and Waves in Solids," Vol. II.

The Δ terms can be written as expansions of the form:

$$\Delta\beta_R = \beta_R(T_0)(\alpha_\beta^{(1)} dT + \alpha_\beta^{(2)} dT^2 + \alpha_\beta^{(3)} dT^3) \quad (A-3)$$

$$\Delta\rho = \rho(T_0)(\alpha_\rho^{(1)} dT + \alpha_\rho^{(2)} dT^2 + \alpha_\rho^{(3)} dT^3) \quad (A-4)$$

$$= \rho^{(1)} dT + \rho^{(2)} dT^2 + \rho^{(3)} dT^3 \quad (A-5)$$

$$\Delta c_{ijkl} = c_{ijkl}^{(1)} dT + c_{ijkl}^{(2)} dT^2 + c_{ijkl}^{(3)} dT^3, \text{ etc.} \quad (A-6)$$

to obtain

$$\begin{aligned} \Delta\beta_R &= \beta_R(T_0) (\alpha_\beta^{(1)} dT + \beta_R(T_0) \alpha_\beta^{(2)} dT^2 + \beta_R(T_0) \alpha_\beta^{(3)} dT^3) \\ &= (\omega dT/4P) \int_0^\infty (\rho(T_0) \alpha_\rho^{(1)} |u|^2 + S:c^{(1)}:S + E^* \cdot \epsilon^{(1)} \cdot E \\ &\quad + E^* \cdot e^{(1)} \cdot S + S:e^{(1)} \cdot E) dy \\ &\quad + (\omega dT^2/4P) \int_0^\infty (\rho(T_0) \alpha_\rho^{(2)} |u|^2 + S:c^{(2)}:S + \dots) dy \\ &\quad + (\omega dT^3/4P) \int_0^\infty (\rho(T_0) \alpha_\rho^{(3)} |u|^2 + S:c^{(3)}:S + \dots) dy \end{aligned} \quad (A-7)$$

or

$$\alpha_\beta^{(j)} = (\omega/4P\beta_R(T_0)) \int_0^\infty (\rho(T_0) \alpha_\rho^{(j)} |u|^2 + S:c^{(j)}:S + \dots) dy \quad (A-8)$$

For the problem of quartz, the electrostatic coupling is small and the electric terms can be ignored. Thus Δd and $\Delta \epsilon$ in (A-8) may be set to zero resulting in the simplified equation.

$$\alpha_\beta^{(j)} = (\omega/4P\beta_R) \int_0^\infty (\rho(T_0) \alpha_\rho^{(j)} |u|^2 + S:c^{(j)}:S) dy \quad (A-9)$$

The integrals are calculable, for instance, from (14),

$$\begin{aligned} &\int_0^\infty \rho(T_0) \alpha_\rho^{(1)} |u|^2 dy \\ &= \rho(T_0) \alpha_\rho^{(1)} \sum_n \int_0^\infty \left[\sum_m C_m \alpha_i^{(m)} \exp(-i \beta_R b^{(m)} y) \right] \\ &\quad \left[\sum_n C_n^* \alpha_i^{(n)*} \exp(i \beta_R b^{(n)} y) \right] dy \end{aligned} \quad (A-10)$$

The problem can easily be extended to multi-layered media by simply performing the integral over each layer separately. For the double layer (A-9) becomes:

$$\int_0^{\alpha} \rho_1(T_0) \alpha_{\rho_1}^{(1)} |u|^2 dy + \int_{\alpha}^{\infty} \rho_2(T_0) \alpha_{\rho_2}^{(2)} |u|^2 dy + \dots \quad (\text{A-11})$$

Because the dependence of u , is given explicitly by (13), it is not necessary to use numerical integration procedures, as demonstrated in (A-10).

Once the $\alpha_{\beta}^{(i)}$ have been calculated from (A-9) the $\alpha_v^{(i)}$ are simply determined. Using $\beta = \omega/V_*$, and (A-9) we determine $\alpha_F^{(i)}$.

APPENDIX B

VOLUME PERTURBATION FORMULA OF SINHA AND TIERSTEN

The approach used by Sinha and Tiersten includes the effects of distortion caused by heating a substrate of quartz and is based in the coordinate system to which the fundamental elastic constants refer. In this reference system, the density is constant and the $\alpha_i^{(i)}$ are equivalent to the $\alpha_i^{(i)}$.

In this new reference system, the perturbation formula becomes¹

$$(\Delta v/v_s) = (1/2\beta_R^2 v^2) (H/N^2), \quad (B-1)$$

$$N^2 = (\rho^0 \pi i / \beta_R^2) \sum_{m=1}^4 \sum_{n=1}^4 (c^{(m)} \alpha^{(m)} c^{(n)*} \alpha^{(n)*}) / (\beta_m - \beta_n^*) \quad (B-2)$$

$$H = - \int_0^\infty dy \int_{-\pi/\beta_R}^{\pi/\beta_R} dz (K_{zz} u_{z,z} + K_{zy} u_{y,z} + K_{zx} u_{z,x} + K_{yz} u_{z,y} + K_{yy} u_{y,y} + K_{yx} u_{x,y}) \quad (B-3)$$

$$K_{L\gamma} = (c_{L\gamma M\alpha} + \Delta c_{L\gamma M\alpha}) u_{\alpha, M} \quad (B-4)$$

For the first order perturbation in T we have:

$$c_{L\gamma M\alpha} = (c_{L\gamma M\nu AB} \alpha_{AB} + c_{L\gamma KM} \alpha_{\nu K} + c_{LKM\nu} \alpha_{\gamma K}) dT \quad (B-5)$$

$$\Delta c_{L\gamma M\alpha} = (d c_{L\gamma M\alpha} / dT) dT \quad (B-6)$$

Where $c_{L\gamma M\alpha}$ are the second order elastic constants previously denoted simply as $c_{L\gamma M\alpha}$ and $c_{L\gamma M\nu AB}$ are the third order elastic constants. The terms $\Delta c_{L\gamma M\alpha}$ as calculated by Tiersten² is available only to first order in T, and the higher order elastic constants $c_{L\gamma M\nu ABCD}$ have never been determined.

¹"On The Temperature Dependence Of The Velocity Of Surface Waves On Quartz," B.K. Sinha and H.F. Tiersten, 1978 Ultrasonics Symposium Proceeding, IEEE, pp. 662-665.

²"Temperature dependence of the Fundamental Elastic Constants of Quartz," B.K. Sinha and H.F. Tiersten, Proceedings of the 32nd Annual Symposium on Frequency Control, 1978, pp. 150-153.

APPENDIX C

THE DIFFERENTIATION METHOD

A method for determining the theoretical temperature dependence of Rayleigh Surface Waves consists of formally differentiating the wave equation and boundary conditions. The boundary conditions and wave equation must be true at all temperatures, placing restraints on how the parameters of the wave equation may vary. In this technique, the derivatives of these equations with respect to temperature are set to zero and solved for the velocity temperature dependence. This method follows the methods used by Bechmann, Ballato, and Lukaszek¹ to compute the temperature dependence of the fundamental elastic constants from frequency data, except that the simplifying assumptions of assuming bulk wave solutions cannot be made. This method was later used by Hauden² to search for temperature stable cuts of quartz.

Christoffel's wave equation can be written in matrix form as

$$\begin{bmatrix} \Gamma_{11} - \rho V_s^2 & \Gamma_{12} & \Gamma_{13} & \Gamma_{14} \\ \Gamma_{12} & \Gamma_{22} - \rho V_s^2 & \Gamma_{23} & \Gamma_{24} \\ \Gamma_{13} & \Gamma_{23} & \Gamma_{33} - \rho V_s^2 & \Gamma_{34} \\ \Gamma_{14} & \Gamma_{24} & \Gamma_{34} & \Gamma_{44} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} = 0 \quad (C-1)$$

where

$$\begin{aligned} \Gamma_{11} &= c_{55} b^2 + 2c_{15} b + c_{11} & \Gamma_{23} &= c_{34} b^2 + (c_{36} + c_{45}) b + c_{56} \\ \Gamma_{22} &= c_{44} b^2 + 2c_{46} b + c_{66} & \Gamma_{44} &= -(e_{33} b^2 + 2e_{13} b + e_{11}) \\ \Gamma_{33} &= c_{33} b^2 + 2c_{35} b + c_{55} & \Gamma_{14} &= e_{35} b^2 + (e_{15} + e_{31}) b + e_{11} \\ \Gamma_{12} &= c_{45} b^2 + (c_{14} + c_{56}) b + c_{16} & \Gamma_{24} &= e_{34} b^2 + (e_{14} + e_{36}) b + e_{16} \\ \Gamma_{13} &= c_{35} b^2 + (c_{13} + c_{55}) b + c_{15} & \Gamma_{34} &= e_{33} b^2 + (e_{13} + e_{35}) b + e_{15} \end{aligned} \quad (C-2)$$

¹"Higher Order Temperature Coefficients of the Elastic Stiffnesses and Compliances of Alpha Quartz," Bechmann, Ballato, and Lukaszek, Proc. IRE, Aug 1962, pp. 1812-1822.

²"Higher Order Temperature Coefficients of Quartz SAW Oscillators," D. Handen, M. Michael, J.J. Gagnepain, Proc. Frequency Control Symposium (1978), pp. 77-86.

following the notation used in the previous section and in Matthews¹. This equation holds for each of the four modes, hereafter designated by a superscript m.

The boundary conditions become, in matrix form,

$$\begin{bmatrix} \dots (C_{33,1} + C_{33,3} b^{(m)}) \alpha_1^{(m)} + (e_{133} + e_{333} b^{(m)}) \alpha_4^{(m)} \dots \\ \dots (C_{31,1} + C_{31,3} b^{(m)}) \alpha_1^{(m)} + (e_{131} + e_{331} b^{(m)}) \alpha_4^{(m)} \dots \\ \dots (C_{32,1} + C_{32,3} b^{(m)}) \alpha_1^{(m)} + (e_{132} + e_{332} b^{(m)}) \alpha_4^{(m)} \dots \\ \dots (e_{31,1} + e_{31,3} b^{(m)}) \alpha_1^{(m)} - (e_{31} + e_{33} b^{(m)} - i\epsilon_0) \alpha_4^{(m)} \dots \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{bmatrix} = 0 \quad (C-3)$$

where only the m'th column is shown and the C_m 's are the amplitudes of each mode. This formulation assumes a normalization of the α 's

$$(\alpha_1^{(m)})^2 + (\alpha_2^{(m)})^2 + (\alpha_3^{(m)})^2 + (\alpha_4^{(m)})^2 = 1. \quad (C-4)$$

The first condition we can place on the wave equation is that the determinant of Christoffel's equation vanishes for all temperature, or

$$d/dT \begin{vmatrix} \Gamma_{11} - \rho V_s^2 & \Gamma_{12} & \Gamma_{13} & \Gamma_{14} \\ \Gamma_{12} & \Gamma_{22} - \rho V_s^2 & \Gamma_{23} & \Gamma_{24} \\ \Gamma_{13} & \Gamma_{23} & \Gamma_{33} - \rho V_s^2 & \Gamma_{34} \\ \Gamma_{14} & \Gamma_{24} & \Gamma_{34} & \Gamma_{44} \end{vmatrix} = 0 \quad (C-5)$$

For each of the four modes, this equation is valid, resulting in four equations in five unknowns, dV_s/dT , and $db^{(m)}/dT$ of the form $F_1^{(m)}(dV_s/dT, db^{(m)}/dT) = 0$, $m = 1, 2, 3, 4$.

For each mode, Christoffel's matrix equation (C-1) must vanish, yielding the set of equations

$$\begin{aligned} (d/dT) (\alpha_1^{(m)} (\Gamma_{11}^{(m)} - \rho V_s^2) + \alpha_2^{(m)} \Gamma_{12}^{(m)} + \alpha_3^{(m)} \Gamma_{13}^{(m)} + \alpha_4^{(m)} \Gamma_{14}^{(m)}) &= 0 \\ (d/dT) (\alpha_1^{(m)} \Gamma_{12}^{(m)} + \alpha_2^{(m)} (\Gamma_{22}^{(m)} - \rho V_s^2) + \alpha_3^{(m)} \Gamma_{23}^{(m)} + \alpha_4^{(m)} \Gamma_{24}^{(m)}) &= 0 \\ (d/dT) (\alpha_1^{(m)} \Gamma_{13}^{(m)} + \alpha_2^{(m)} \Gamma_{23}^{(m)} + \alpha_3^{(m)} (\Gamma_{33}^{(m)} - \rho V_s^2) + \alpha_4^{(m)} \Gamma_{34}^{(m)}) &= 0 \\ (d/dT) (\alpha_1^{(m)} \Gamma_{14}^{(m)} + \alpha_2^{(m)} \Gamma_{24}^{(m)} + \alpha_3^{(m)} \Gamma_{34}^{(m)} + \alpha_4^{(m)} \Gamma_{44}^{(m)}) &= 0. \end{aligned} \quad (C-6)$$

This results in 16 equations (four per mode) and an additional 16 unknowns (the $\alpha_i^{(m)}$'s) of the form

$$F_{2i}^{(m)}(dV_s/dT, db^{(m)}/dT, d\alpha_1^{(m)}/dT, d\alpha_2^{(m)}/dT, d\alpha_3^{(m)}/dT, d\alpha_4^{(m)}/dT) = 0$$

¹"Surface Wave Filters," H. Matthews, John Wiley and Sons, New York (1977).

Using (C-3) we obtain the single equation

$$(d/dt) \begin{vmatrix} \dots\dots (c_{3311} + c_{3313}b^{(m)}) \alpha_1^{(m)} + (e_{133} + e_{333}b^{(m)}) \alpha_4^{(m)} \dots\dots \\ \dots\dots (c_{3111} + c_{3113}b^{(m)}) \alpha_1^{(m)} + (e_{131} + e_{331}b^{(m)}) \alpha_4^{(m)} \dots\dots \\ \vdots \\ \vdots \\ \vdots \end{vmatrix} = 0 \quad (C-7)$$

of the form $F_1^{(m)} (db^{(1)}/dT, db^{(2)}/dT, \dots, d\alpha_1^{(m)}/dT) = 0$

and four equations of the form

$$(d/dT) \sum_m C_m [(c_{3311} + c_{3313}b^{(m)}) \alpha_1^{(m)} + (e_{133} + e_{333}b^{(m)}) \alpha_4^{(m)}] = 0 \quad (C-8)$$

$$(d/dT) \sum_m C_m [(c_{3111} + c_{3113}b^{(m)}) \alpha_1^{(m)} + (e_{131} + e_{331}b^{(m)}) \alpha_4^{(m)}] = 0$$

of the form $F_4^{(m)} (db^{(m)}/dT, d\alpha_1^{(m)}/dT, dC_m/dT) = 0 \quad (C-9)$

From (5) $\alpha_1^{(m)} (d\alpha_1^{(m)}/dT) + \alpha_2^{(m)} (d\alpha_2^{(m)}/dT) + \alpha_3^{(m)} (d\alpha_3^{(m)}/dT) \quad (C-10)$

$$+ \alpha_4^{(m)} (d\alpha_4^{(m)}/dT) = 0$$

or

$$F_5^{(m)} (d\alpha_1^{(m)}/dT) = 0 \quad (C-11)$$

Combining the above results gives 25 equations in the 25 unknowns.

$$dV_s/dT, db^{(m)}/dT, d\alpha_1^{(m)}/dT, dC_m/dT$$

which are solved simultaneously. Once the temperature dependence of the Rayleigh wave velocity is found, the frequency dependence is found in the usual way.

To obtain the second order dependence of V_s , the 25 equations are differentiated again. The values of $dV_s/dT, db^{(m)}/dT, d\alpha_1^{(m)}/dT$ and dC_m/dT previously obtained are used to obtain d^2V_s/dT^2 , etc.

APPENDIX D

SOLUTION METHOD

Calculating the velocity of a Rayleigh wave requires a complete solution of the problem to be performed. All of the constants in equation (13) must be evaluated. The standard used at Motorola as developed by Campbell and Jones is outlined below.

First the fundamental constants are rotated into the coordinate system of interest.

Next a value of V_r is picked. The coefficients τ_{ij} of equation (C-2) are evaluated and the determinant of the matrix in equation (C-1) is set to zero, as it must be if a solution of (C-1) is to be found. This results in an eighth order equation in b . This equation is solved for the eight complex roots. The four roots $b^{(m)}$ in the lower complex plane are retained, the four discarded roots not satisfying the boundary conditions at infinity. Equation (C-1) is then solved for the four eigenvectors $\alpha_i^{(m)}$. The $b_i^{(m)}$ and the corresponding eigenvector $\alpha_i^{(m)}$ are substituted into equation (C-3) and the determinant of the matrix in equation (C-3) is evaluated. This determinant must be zero for a solution to (C-3) exist. If it is not zero, V_r is varied, and the whole procedure repeated, until it is. Once a value of V_r is found such that the determinant in equation (C-3) vanishes, the solution to (C-3) is found, giving the values for C_m . These constants completely describe the solution of equation (13), as well as providing the exact velocity.

APPENDIX E

EQUIVALENCE OF TEMPERATURE COEFFICIENTS OF FREQUENCY AND DELAY

In the following section, the relations relating the first, second, and third order temperature coefficients of delay and frequency will be derived. These relations show implicitly the equivalence of each representation of the device temperature characteristics, and justify their interchangeable usage.

In the text, we have used the following notation:

$$\tau = \text{delay time of delay line oscillator} \quad (\text{E-1})$$

$$i\text{th order temperature coefficient of delay} = \text{TCD}^{(i)} = \alpha_{\tau}^{(i)} \quad (\text{E-2})$$

$$F = \text{frequency of delay line oscillator} \quad (\text{E-3})$$

$$i\text{th order temperature coefficient of frequency} = \alpha_F^{(i)} \quad (\text{E-4})$$

$$\tau = \tau_0 (1 + \alpha_{\tau}^{(1)} (T - T_0) + \alpha_{\tau}^{(2)} (T - T_0)^2 + \alpha_{\tau}^{(3)} (T - T_0)^3 + \dots) \quad (\text{E-5})$$

$$F = F_0 (1 + \alpha_F^{(1)} (T - T_0) + \alpha_F^{(2)} (T - T_0)^2 + \alpha_F^{(3)} (T - T_0)^3 + \dots) \quad (\text{E-6})$$

where T is temperature and T_0 is a reference temperature, 25°C in our case. For a SAW oscillator, $F\tau = \text{constant}$ or

$$\begin{aligned} \tau/\tau_0 &= F_0/F \\ &= 1/(1 + \alpha_F^{(1)} (T - T_0) + \alpha_F^{(2)} (T - T_0)^2 + \alpha_F^{(3)} (T - T_0)^3 + \dots) \end{aligned} \quad (\text{E-7})$$

Using the relation

$$1/(1 + X) \cong 1 - X + X^2 - X^3 \text{ for } X \ll 1 \quad (\text{E-8})$$

we can write

$$\begin{aligned} \tau/\tau_0 &= 1 - [\alpha_F^{(1)} (T - T_0) + \alpha_F^{(2)} (T - T_0)^2 + \alpha_F^{(3)} (T - T_0)^3] \\ &\quad + [(\alpha_F^{(1)} (T - T_0))^2 + 2\alpha_F^{(1)} (T - T_0) \alpha_F^{(2)} (T - T_0)^2] \\ &\quad - [\alpha_F^{(1)} (T - T_0)]^3 + \text{higher order terms} \end{aligned} \quad (\text{E-9})$$

$$= 1 - \alpha_F^{(1)} (T - T_0) + (-\alpha_F^{(2)} + (\alpha_F^{(1)})^2) (T - T_0)^2 + (-\alpha_F^{(3)} + 2\alpha_F^{(1)} \alpha_F^{(2)} - (\alpha_F^{(1)})^3) (T - T_0)^3 \quad (\text{E-10})$$

Equating powers of $T - T_0$ in (E-5) and (E-10), we obtain

$$\alpha_T^{(1)} = -\alpha_F^{(1)} \quad (E-11)$$

$$\alpha_T^{(2)} = -\alpha_F^{(2)} + (\alpha_F^{(1)})^2 \quad (E-12)$$

$$\alpha_T^{(3)} = -\alpha_F^{(3)} + 2\alpha_F^{(1)}\alpha_F^{(2)} - (\alpha_F^{(1)})^3 \quad (E-13)$$

As the only assumption on F and τ used is that of equation (E-7) which is symmetric in F and τ , we immediately obtain

$$\alpha_F^{(1)} = -\alpha_T^{(1)} \quad (E-14)$$

$$\alpha_F^{(2)} = -\alpha_T^{(2)} + (\alpha_T^{(1)})^2 \quad (E-15)$$

$$\alpha_F^{(3)} = -\alpha_T^{(3)} + 2\alpha_T^{(1)}\alpha_T^{(2)} - (\alpha_T^{(1)})^3 \quad (E-16)$$

Using (E-11) through (E-16), we can always relate one set of temperature coefficients to the other.

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MOTOROLA INC SCOTTSDALE ARIZ GOVERNMENT ELECTRONICS DIV F/G 20/2
DOUBLY ROTATED CUT SAW DEVICES.(U)
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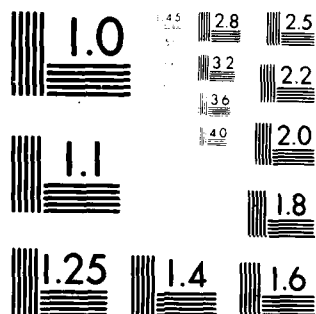
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APPENDIX F

X-RAY RUN

The following is an example of the computer results from the FORTRAN X-ray orientation computer program for the doubly rotated cut 7/27/0. File MILDAT contains only the two Miller indices shown on the printout on this run.

10103 APR 10 '60 1000047
 JOB 530, WILLIAMS(3523200), 7, FILE=RAYJOB, ID=03, LINE=22
 LIMIT (TIME, 2), (CO, 30), (UO, 30)
 ASSIGN P1103, (FILE, MILDAT), (IN)
 ASSIGN P1104, (FILE, ERRDAT), (IN)
 RUN (LMN, XRAYLM)
 INPUT THE THREE ANGLES PHI, THETA, PSI

***** ANGLES ARE (YXHLT) 7.00000 (0 MIN.) / 27.0000 (0 MIN.) / .000000 (0 MIN.)

 MILLER INDICES: 0 -1 1

NORMAL VECTOR = .95754E-01 -.975690 .197133
 THETA= 13.3213

PLATE IN POSITION 1 (-1 AXIS VERTICAL, 2 AXIS NORMAL)
 G = ANGLE OF INCIDENCE: 24.0044 (48 MIN.)
 BETA= 2.52901 (32 MIN.)
 G PLUS G PRIME= EXIT ANGLE: 126.5310 (32 MIN.)
 INTENSITY FACTOR: .709521E-01 INTENSITY: .000000

PLATE IN POSITION 3 (1 AXIS VERTICAL, 2 AXIS NORMAL)
 G = ANGLE OF INCIDENCE: 11.96138 (58 MIN.)
 BETA= 2.52901 (32 MIN.)
 G PLUS G PRIME= EXIT ANGLE: 126.5310 (32 MIN.)
 INTENSITY FACTOR: .924245 INTENSITY: .000000

 MILLER INDICES: 0 -2 1

NORMAL VECTOR = .113399 -.980196 -.929136E-01
 THETA= 22.8995

PLATE IN POSITION 2 (-3 AXIS VERTICAL, 2 AXIS NORMAL)
 G = ANGLE OF INCIDENCE: 29.5443 (33 MIN.)
 BETA= 1.4657 (9 MIN.)
 G PLUS G PRIME= EXIT ANGLE: 145.6526 (39 MIN.)
 INTENSITY FACTOR: .362103 INTENSITY: .000000

PLATE IN POSITION 4 (3 AXIS VERTICAL, 2 AXIS NORMAL)
 G = ANGLE OF INCIDENCE: 16.4650 (28 MIN.)
 BETA= 4.14637 (9 MIN.)
 G PLUS G PRIME= EXIT ANGLE: 145.6526 (39 MIN.)
 INTENSITY FACTOR: .633495 INTENSITY: .000000

```

*****
LAUE ANGLES DEFINED SUCH THAT ALPHA = ANGLE FROM BEAM,
BETA = ROTATION CLOCKWISE FROM P1, DIST TO CRYSTAL = 10.0000
MILLER INDICES: 0 -1 1 LAUE SPOT ANGLES: ALPHA=25.3188 BETA=64.0927 X=2.06704 Y=4.25554
MILLER INDICES: 0 -2 1 LAUE SPOT ANGLES: ALPHA=16.0600 BETA=39.3295 X=2.34422 Y=1.92073
*****
LAUE ANGLES DEFINED SUCH THAT ALPHA = ANGLE FROM BEAM,
BETA = ROTATION CLOCKWISE FROM P1.
FOR ROTATIONS E(1) = .000000 E(2) = .000000 E(3) = .000000 ACTUAL ANGLES ARE
(VX=176.99998 (60 MIN.)/27.0000 (60 MIN.)/.000000 ( 0 MIN.))
FOR ROTATIONS E(1) = .500000 E(2) = -.116600 E(3) = .000000 ACTUAL ANGLES ARE
(VX=176.99998 (60 MIN.)/27.5011 (30 MIN.)/.117251 ( 7 MIN.))
*STOP* NORMAL
DATA INFORMATION=IGNORED

```

APPENDIX G

X-RAY PROGRAM

The following is the FORTRAN computer program used to calculate X-ray diffraction angles for a doubly rotated cut of quartz.

15154 APR 18, '80 DC/XRAY.538

1	0,500	COMMON /INTEN/REF
2	1,000	INTEGER M
3	2,000	COMMON /MILLER/M,K,L
4	3,000	COMMON /ERR/EA
5	4,000	DIMENSION EA(3)
6	5,000	CALL CLEAR
7	6,000	CALL ROTATE
8	7,000	CONTINUE
9	8,000	READ(103,10,END=99)M,K,L,REF
10	9,000	CALL NORMAL(1ERR)
11	10,000	CALL SPOTS
12	11,000	IF(1ERR.EQ.0)CALL GONIOH
13	12,000	GOTO 20
14	13,000	CONTINUE
15	14,000	CALL LAST
16	15,000	CONTINUE
17	16,000	READ(104,30,END=99)1EA(1),EA(2),EA(3)
18	17,000	CALL ERROR
19	18,000	GOTO 9A
20	19,000	FORMAT(30)
21	20,000	FORMAT(32,6)
22	21,000	STOP 'NORMAL'
23	22,000	END
24	23,000	SUBROUTINE ROTATE
25	24,000	REAL R(3,3)
26	25,000	COMMON /ROT/R
27	26,000	COMMON /ANGLE/A1,A2,A3
28	27,000	CALL BCFUN(A1,B1,C1)
29	28,000	CALL BCFUN(A2,B2,C2)
30	29,000	CALL BCFUN(A3,B3,C3)
31	30,000	R(1,1)=C1-C3-B1-B2-B3
32	31,000	R(1,2)=B1-C3-C1-B2-B3
33	32,000	R(1,3)=C2-B3
34	33,000	R(2,1)=B1-C2
35	34,000	R(2,2)=C1-C2
36	35,000	R(2,3)=B2
37	36,000	R(3,1)=C1-B3-B1-B2-C3
38	37,000	R(3,2)=B1-B3-C1-B2-C3
39	38,000	R(3,3)=C2-C3
40	39,000	RETURN
41	40,000	END

```

41,000 SUBROUTINE CLEAR
42,000 COMMON/CLEAR/N
43,000 COMMON /ANGLE/A1,A2,A3
44,000 NSU
45,000
46,000 WRITE(100,10)
47,000 FORMAT(' INPUT THE THREE ANGLES PHI,THETA,PBI')
48,000 READ(105,30)A1,A2,A3
49,000
50,000 FORMAT(36)
51,000 WRITE(100,20)A1,M1(A1),A2,M1(A2),A3,M1(A3)
52,000
53,000 FORMAT('1 ***** ANGLES ARE,
54,000 * (XWLT),*,*, (*,12,*, MIN.),*,*, (*,12,*, MIN.),*,*, (*,12,
55,000 * MIN.),*,*)
56,000 RETURN
57,000
58,000 END
59,000
60,000 SUBROUTINE NORMAL(IERR)
61,000 INTEGER M
62,000 COMMON /RNT/R
63,000 COMMON /NORM/RN,THETA
64,000 COMMON /MILLER/M,K,L
65,000 REAL RN(3),RNI(3),R(3,3)
66,000 IERR=0
67,000
68,000 RNI(1)=RN
69,000 RNI(2)=FLOAT(M+2*K)/SQRT(3.0)
70,000 RNI(3)=FLOAT(L)/1.09997
71,000
72,000 DO 10 I=1,3
73,000 R=RN(RNI(I)+RNI(I))
74,000 R=SQRT(R)
75,000
76,000 DO 20 I=1,3
77,000 RNI(I)=RNI(I)/R
78,000
79,000 DO 30 I=1,3
80,000 RN(I)=0.
81,000
82,000 DO 30 J=1,3
83,000 R=RN(I)+RN(J)+RNI(J)
84,000 R=SQRT(R)
85,000
86,000 CDIV=1.09997
87,000 D=AO/(SQRT((4./3.)*FLOAT(M+M+K+K+K)+FLOAT(L+L+L)/(CDIV+CDIV+CDIV)))
88,000
89,000 PLAND=1.5376
90,000 IF (PLAND*.65,2.0+ABS(D)) GO TO 40
91,000 THETA=ASIN(PLAND/A/(2.*D))
92,000 THETA=THETA+100./3.141592654
93,000 RETURN
94,000 CONTINUE

```

```

83,000 IERR=1
84,000 RETURN
85,000 END
86,000 SUBROUTINE SPOTS
87,000 COMMON /CLEAN/N
88,000 DIMENSION IREM(3,250),REM(2,250)
89,000 INTEGER N
90,000 COMMON /NORM/RN,THETA
91,000 COMMON /MILLER/M,K,L
92,000 REAL RN(3)
93,000 HERE WE USE TWICE THE VALUE PUT IN BY WEISING, WHICH HE TAKES
94,000 INTO ACCOUNT BY USE OF HIS SPECIAL SCALE ON THE FILM ITSELF.
95,000 ALPHA=2.0*ACOS(-RN(2))/100./3.141592654
96,000 IF(ABS(ALPHA).GT.60.)RETURN
97,000 BETAS=0.
98,000 IF(RN(3).LT.0)BETAS=90.
99,000 IF(RN(1).EQ.0.)GO TO 10
100,000 BETAS=ATAN(RN(3)/RN(1))+100./3.141592654
101,000 CONTINUE
102,000
103,000 10
104,000 N=N+1
105,000 IF(N.GT.250)STOP'ARRAY SIZE TOO SMALL'
106,000 IREM(1,N)=H
107,000 IREM(2,N)=K
108,000 IREM(3,N)=L
109,000 REM(1,N)=ALPHA
110,000 REM(2,N)=BETAS
111,000 RETURN
112,000 ENTRY LAST
113,000 DIST=10.0
114,000 WRITE(100,40)DIST
115,000 FORMAT('1' //)
116,000 * LAUE ANGLES DEFINED SUCH THAT ALPHA & ANGLE FROM BEAM = *
117,000 * BETA & ROTATION CLOCKWISE FROM P1, DIST TO CRYSTAL = *C)
118,000 DO 30 I=1,N
119,000 CALL SCFUN(REM(1,I),ALB,ALC)
120,000 CALL SCFUN(REM(2,I),BEB,BEC)
121,000 ALTB=ALB/ALC
122,000 X=DIST*ALTB*BEC
123,000 Y=DIST*ALTB*BEC
124,000 WRITE(100,20)(IREM(J,I),J=1,3),REM(1,I),REM(2,I),X,Y
125,000 CONTINUE
126,000 WRITE(100,41)
127,000 FORMAT('1' //)

```

```

120 - 110.000
121 - 110.000
122 - 120.000
123 - 121.000
124 - 122.000
125 - 123.000
126 - 124.000
127 - 125.000
128 - 126.000
129 - 127.000
130 - 128.000
131 - 129.000
132 - 130.000
133 - 131.000
134 - 131.100
135 - 131.150
136 - 131.200
137 - 131.300
138 - 131.400
139 - 131.500
140 - 132.000
141 - 133.000
142 - 134.000
143 - 135.000
144 - 136.000
145 - 137.000
146 - 138.000
147 - 139.000
148 - 140.000
149 - 141.000
150 - 142.000
151 - 143.000
152 - 144.000
153 - 145.000
154 - 146.000
155 - 147.000
156 - 148.000
157 - 149.000
158 - 150.000
159 - 151.000
160 - 152.000
161 - 153.000

```

```

** LAUE ANGLES DEFINED SUCH THAT ALPHA = ANGLE FROM BEAM.0.0.
** RETA = ROTATION COUNTERWISE FROM P1.0
FORMAT(, MILLER INDICES1,3(I2,I3),, LAUE SPOT ANGLES: ALPHA0,
+G,, RETA0,G,, X0,G,, Y0,G)
RETURN
END
SUBROUTINE GONIOM
  COMMON /INTFN/REF
  COMMON /MILLER/M,K,L
  COMMON /MORR/RN,THETA
  LOGICAL NO1,NO2,NO3,NO4
  DIMENSION RN(3)
  DATA PHI/3.141592654/,RETMAX/5.0/
  IF(ABS(RN(2)).LT. 0.9)RETURN
  IF(L.GT.0)GOTO 12
  IF(L.LT.0)RETURN
  IF(K.GT.0)GOTO 12
  IF(K.EQ.0 .AND. M.GT.0)GOTO 12
  RETURN
CONTINUE
NO1=.TRUE.
NO2=.TRUE.
CALL SCFUN(THETA,TTS,TTC)
T1=2.*TTS/RN(1)
T2=2.*TTS/RN(3)
IF(ABS(T1).GT.1.0)NO1=.FALSE.
IF(ABS(T2).GT.1.0)NO2=.FALSE.
IF(NO1)RET1=180.*ASIN(T1)/PHI
IF(NO2)RET2=180.*ASIN(T2)/PHI
IF(ABS(RET1).GT.RETMAX)NO1=.FALSE.
IF(ABS(RET2).GT.RETMAX)NO2=.FALSE.
IF(.NOT.NO1 .AND. .NOT.NO2)RETURN
DELTP1=180.*ATAN(RN(3)/RN(2))/PHI
DELTP2=180.*ATAN(RN(1)/RN(2))/PHI
T=180.*ASIN(RN(1)/PHI)
CALL SCFUN(THETA,TTS,TTC)
T=TTS/TTC
IF(ABS(T).GT.1.0)NO1=.FALSE.
IF(NO1)THETP=180.*ASIN(T)/PHI
T=180.*ASIN(RN(3)/PHI)
CALL SCFUN(T,TTS,TTC)

```

```

171 - 154,000
172 - 155,000
173 - 156,000
174 - 157,000
175 - 158,000
176 - 159,000
177 - 160,000
178 - 161,000
179 - 162,000
180 - 163,000
181 - 164,000
182 - 165,000
183 - 166,000
184 - 167,000
185 - 168,000
186 - 169,000
187 - 170,000
188 - 171,000
189 - 172,000
190 - 173,000
191 - 174,000
192 - 175,000
193 - 176,000
194 - 177,000
195 - 178,000
196 - 179,000
197 - 180,000
198 - 181,000
199 - 182,000
200 - 183,000
201 - 184,000
202 - 185,000
203 - 186,000
204 - 187,000
205 - 188,000
206 - 189,000
207 - 190,000
208 - 191,000
209 - 192,000
210 - 193,000
211 - 194,000
212 - 195,000
213 - 196,000

TBTB/TC
IF(ABS(T).GT.1.0)NO2=.FALSE.
IF(N02)THETP=180.*ABSIN(T)/PHI
G1=THETP-DELTP1
G2=THETP+DELTP2
G3=THETP-DELTP1
G4=THETP+DELTP2
CALL SCFUN(2.*THETA,T8,TC)
CALL SCFUN(BE1,T9,TC)
IF(ABS(TC/TC).GT.1.0)NO1=.FALSE.
IF(N01)GPP1=180.*ACOS(TC/TC)/PHI
CALL SCFUN(BE2,T9,TC)
IF(ABS(TC/TC).GT.1.0)NO2=.FALSE.
IF(N02)GPP2=180.*ACOS(TC/TC)/PHI
IF(.NOT.N01 .AND. .NOT.N02)RETURN
NO3=N01
NO4=N02
IF(G1.LT.0. .OR. GPP1.LT.61)NO1=.FALSE.
IF(G2.LT.0. .OR. GPP2.LT.62)NO2=.FALSE.
IF(G3.LT.0. .OR. GPP1.LT.63)NO3=.FALSE.
IF(G4.LT.0. .OR. GPP2.LT.64)NO4=.FALSE.
CALL SCFUN(2.*THETA-G1,T9,TC)
CALL SCFUN(G1-G8,GC)
FACT1=TS/(TS-G8)
CALL SCFUN(2.*THETA-G2,T9,TC)
CALL SCFUN(G2-G8,GC)
FACT2=TS/(TS-G8)
CALL SCFUN(2.*THETA-G3,T9,TC)
CALL SCFUN(G3-G8,GC)
FACT3=TS/(TS-G8)
CALL SCFUN(2.*THETA-G4,T9,TC)
CALL SCFUN(G4-G8,GC)
FACT4=TS/(TS-G8)
IF(FACT1.LT.0. .OR. FACT1.GT.1.0)NO1=.FALSE.
IF(FACT2.LT.0. .OR. FACT2.GT.1.0)NO2=.FALSE.
IF(FACT3.LT.0. .OR. FACT3.GT.1.0)NO3=.FALSE.
IF(FACT4.LT.0. .OR. FACT4.GT.1.0)NO4=.FALSE.
IF(.NOT.N01 .AND. .NOT.N02 .AND. .NOT.N03 .AND. .NOT.N04)RETURN
WRITE(106,10)M,K,L
10 FORMAT(' ',10X,M,K,L)
10
WRITE(106,20)(RN(I),I=1,3),THETA
20
FORMAT(' NORMAL VECTOR ',3G,/,', THETA ',G)
20
FORMAT(' PLATE IN POSITION ',11,') (' ,
100

```

```

214 - 186,000
215 - 187,000
216 - 188,000
217 - 189,000
218 - 190,000
219 - 191,000
220 - 192,000
221 - 193,000
222 - 194,000
223 - 195,000
224 - 196,000
225 - 197,000
226 - 198,000
227 - 199,000
228 - 200,000
229 - 201,000
230 - 202,000
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243 - 215,000
244 - 216,000
245 - 217,000

110
+12,° AXIS VERTICAL, 2 AXIS NORMAL)°)
FOR-MAT(° G ° ANGLE OF INCIDENCE,° G,° ('12,° MIN.),°)
+° BET1,° G,° ('12,° MIN.),°)
+° G PLUS G PRIMEEXIT ANGLE,° G,° ('12,° MIN.),°)
+° INTENSITY FACTOR,° G,° INTENSITY,° G)
IF(N01)WRITE(108,100)1,-1
IF(N01)WRITE(108,110)G1,MI(G1),BET1,MI(BET1),GPP1,MI(GPP1),FACT1
+REF+FACT1
IF(N02)WRITE(108,100)2,-3
IF(N02)WRITE(108,110)G2,MI(G2),BET2,MI(BET2),GPP2,MI(GPP2),FACT2
+REF+FACT2
IF(N03)WRITE(108,100)3,1
IF(N03)WRITE(108,110)G3,MI(G3),-BET1,MI(-BET1),GPP1,MI(GPP1),
+FACT3,REF+FACT3
IF(N04)WRITE(108,100)4,3
IF(N04)WRITE(108,110)G4,MI(G4),-BET2,MI(-BET2),GPP2,MI(GPP2),
+FACT4,REF+FACT4
RETURN
END
INTEGER FUNCTION MI(X)
REAL X,X1
X1=ABS(X)
MI=INT(66.0*(X1-INT(X1))+.5)
RETURN
END
SUBROUTINE ERROR
COMMON /ERR/EA
COMMON /RNT/H
DIMENSION EA(3),R(3,3),ES(3)
DATA PH1/3.141592654/
DO 10 I=1,3
CALL SCFUN(EA(I),ES(I),T)
T=ER(2,2)-ES(1)*R(3,2)+ES(3)*R(2,1)
T1=ER(2,1)-ES(1)*R(3,1)+ES(3)*R(1,1)
A1=90
IF(T.NE.0.)A1=180.-ATAN(T1/T)/PHI
T=ER(2,3)-ES(1)*R(3,3)+ES(3)*R(1,3)
A2=180.-ASIN(-T)/PHI
T=ER(3,3)-ES(2)*R(1,3)+ES(1)*R(2,3)
T1=ER(1,3)-ES(3)*R(2,3)+ES(2)*R(3,3)
A3=90
IF(T.NE.0.)A3=180.-ATAN(T1/T)/PHI
WRITE(108,20)(I,EA(I),I=1,3),A1,MI(A1),A2,MI(A2),A3,MI(A3)

```

```

20  FORMAT,' FOR ROTATIONS ',3('E(',11,')' ) = ',6),
*  ACTUAL ANGLES ARE.,/
*,', (YXWLT),6,', (',12,' MIN.),',6,', (',12,' MIN.),',/
*  MIN.),',/
RETURN
END
SUBROUTINE SCFUN(DEC,B,C)
C SIN AND COS OF ANGLE IN DEGREES, EXACT ANG AT 9,180,270,360
X = DEG
IF( X LT. 0.) X = X +360.
IF(X .EQ. 0. .OR. X .EQ.180.) GO TO 150
IF(X .EQ. 90. .OR. X .EQ. 270.) GO TO 200
WAD = X/57.295779
S = SIN(RAD)
C = COS(RAD)
100 RETURN
150 C =1.
S=0.
IF(X .EQ. 180.) C =-1.
GO TO 100
200 S =1.
C =0.
IF(X .EQ. 270.) S =-1.
GO TO 100
END

```

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