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**Program for Calculating X-Ray Powder
Diffraction Interplanar (d) Spacings
with a Tektronix-31 Desk Top
Programmable Calculator**

Ralph R. Eckstein and Yoshio G. Ishida

February 22, 1977

Monsanto

MOUND LABORATORY

Miamisburg, Ohio
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**UNITED STATES ENERGY RESEARCH
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Abstract

A Tektronix-31 (Tektronix Inc. Beaverton, Oregon) desk top calculator program, which is used as a backup to the PDP-8/I computer program, is described. The program yields interplanar (d) spacings and (2θ) angle values from measurements made on an X-ray diffraction film of a powdered sample of a crystalline material. Use of the calculator provides accurate computations in a relatively rapid time interval when the PDP-8/I is not functioning because of downtime for repairs, maintenance, etc.

Introduction

This report relates the capabilities of the Tektronix-31 desk top calculator when used as a backup for the PDP-8/I computer for obtaining accurate and relatively rapid data computations. A program has been written to process line measurements obtained from X-ray powder diffraction films. Essentially, this program is identical in its structure to the one written for use with the PDP-8/I¹ in that it yields interplanar spacings (d-spacings), diffraction angle theta values (2θ), and the camera radius correction factor. Although the Tektronix-31 does compute the data as accurately as does the PDP-8/I, its major shortcomings lie in two areas: the I/O (input/output) of data is slower by a factor of four, and the data presentation is rather bulky and cumbersome to handle. These areas are readily

acceptable, however, when hand calculations are the alternative since the computation of about 40 diffraction lines can be accomplished using the Tektronix-31 calculator in approximately 10 min, whereas hand calculations would require on the order of 4 hr.

The Tektronix-31 has the additional advantage of being capable of transferring data from its memory registers to a tape cassette. This is not only desirable to retain programs for future use; but it is very desirable when the program, as described in this report, is considered. This program, written for X-ray data computation, is composed of 1088 instructions and would be extremely tedious to enter each time it were used without the cassette tape capability.

Mathematical Equations

As in the program written for the PDP-8/I, the equation of prime importance in determining interplanar spacings (d-spacings) and the diffraction angle theta values is the Bragg equation:

$$\lambda = 2d \sin \theta \quad (1)$$

where: λ = wavelength of copper radiation used ($K\alpha_0 = 1.54178 \text{ \AA}$,
 $K\alpha_1 = 1.54051 \text{ \AA}$, $K\alpha_2 = 1.54433$),

d = interplanar spacing

2θ = angle which describes the deviation of diffracted X-rays from the direct beam.

Discussion

This report contains a copy of the machine language program that was written to process a maximum of 60 X-ray powder diffraction line measurements. With some modifications of the R___ registers used,² additional lines could be adequately handled. However, a pattern containing more than 60 different lines is not a common occurrence. As with the use of the PDP-8/I program when the data for more than 60 lines is desired, the input can be divided into two segments and thus adequately handled. Figure 1 shows the program that will routinely process 60 lines of a powder diffraction pattern. Figure 2 shows a simplified version of the flow chart. Figure 3 (Sections A, B, C, and D) shows the flow

chart which is outlined prior to writing the program.

The Tektronix-31 calculator has a maximum of 640 R___ storage registers plus an additional 10 of K_ registers. The R___ registers were not used.² As was previously stated, all of the R___ and K_ registers have not been utilized; and with careful rearrangement, additional storage of data and the computational capabilities of the calculator could be significantly increased.

Presently, the first 360 R___ registers are reserved for data input storage. There are 60 R___ registers reserved to store information about the left line,

0000	EXC_	0063	CLDP	0126	IF 0	0190	0	0254	4	0318	=
0001	ARC_	0064	1	0127	EXC_	0191	PRNT	0255	1	0319	R---
0002	LBL	0065	=	0128	5	0192	EXC_	0256	CLDP	0320	4---
0003	DG/R	0066	R---	0129	CONT	0193	4	0257	+ -	0321	4
0004	CLDP	0067	0	0130	L	0194	B	0258	=	0322	6
0005	P	0068	0	0131	(	0195	(	0259	6	0323	CLDP
0006	R	0069	0	0132	I	0196	I	0260	4	0324	1
0007	O	0070	=	0133	)	0197	)	0261	5	0325	=
0008	G	0071	K_	0134	=	0198	=	0262	9	0326	5
0009	R	0072	3	0135	CLDP	0199	CLDP	0263	6	0327	4
0010	A	0073	=	0136	STOP	0200	STOP	0264	4	0328	0
0011	M	0074	R---	0137	=	0201	=	0265	=	0329	5
0012		0075	4---	0138	R---	0202	R---	0266	R---	0330	1
0013	T	0076	3	0139	R---	0203	R---	0267	4---	0331	=
0014	O	0077	1	0140	0	0204	0	0268	4	0332	R---
0015		0078	CLDP	0141	0	0205	0	0269	2	0333	4---
0016	C	0079	2	0142	0	0206	0	0270	CLDP	0334	4
0017	A	0080	=	0143	PRNT	0207	PRNT	0271	=	0335	7
0018	L	0081	R---	0144	EXC_	0208	EXC_	0272	0	0336	CLDP
0019	C	0082	4---	0145	4	0209	4	0273	7	0337	1
0020		0083	3	0146	M	0210	I	0274	9	0338	=
0021	PAPR	0084	2	0147	(	0211	(	0275	6	0339	5
0022	D	0085	CLDP	0148	I	0212	I	0276	8	0340	4
0023		0086	3	0149	)	0213	)	0277	9	0341	4
0024	S	0087	=	0150	=	0214	=	0278	=	0342	3
0025	P	0088	R---	0151	CLDP	0215	CLDP	0279	R---	0343	3
0026	A	0089	4---	0152	STOP	0216	STOP	0280	4---	0344	=
0027	C	0090	3	0153	=	0217	=	0281	4	0345	R---
0028	I	0091	3	0154	R---	0218	R---	0282	3	0346	4---
0029	N	0092	CLDP	0155	R---	0219	R---	0283	CLDP	0347	4
0030	G	0093	4	0156	0	0220	0	0284	+/-	0348	8
0031	S	0094	=	0157	0	0221	0	0285	=	0349	CLDP
0032		0095	R---	0158	0	0222	0	0286	0	0350	=
0033		0096	4---	0159	PRNT	0223	PRNT	0287	0	0351	R---
0034	PAPR	0097	3	0160	EXC_	0224	EXC_	0288	4	0352	4---
0035	PAPR	0098	4	0161	4	0225	4	0289	6	0353	5
0036	E	0099	CLDP	0162	R	0226	EXC_	0290	7	0354	0
0037	N	0100	5	0163	(	0227	HYP	0291	4	0355	=
0038	T	0101	=	0164	I	0228	LBL	0292	=	0356	R---
0039	E	0102	R---	0165	)	0229	ARC	0293	R---	0357	4---
0040	R	0103	4---	0166	=	0230	1	0294	4---	0358	5
0041		0104	3	0167	CLDP	0231	=	0295	4	0359	1
0042	N	0105	5	0168	STOP	0232	5	0296	4	0360	=
0043	=	0106	CLDP	0169	=	0233	4	0297	CLDP	0361	R---
0044	CLDP	0107	6	0170	R---	0234	1	0298	=	0362	4---
0045	=	0108	=	0171	R---	0235	7	0299	0	0363	5
0046	K_	0109	R---	0172	0	0236	8	0300	0	0364	2
0047	2	0110	4---	0173	0	0237	=	0301	0	0365	=
0048	CLDP	0111	3	0174	0	0238	R---	0302	1	0366	R---
0049	3	0112	6	0175	PRNT	0239	4---	0303	5	0367	4---
0050	6	0113	EXC_	0176	EXC_	0240	4	0304	1	0368	5
0051	5	0114	1	0177	4	0241	0	0305	=	0369	3
0052	=	0115	LBL	0178	C	0242	CLDP	0306	R---	0370	EXC
0053	R---	0116	1	0179	(	0243	1	0307	4---	0371	DG/R
0054	3	0117	38M2	0180	I	0244	=	0308	4	0372	LBL
0055	6	0118	K_	0181	)	0245	5	0309	5	0373	HYP
0056	5	0119	2	0182	=	0246	7	0310	CLDP	0374	R---
0057	CLDP	0120	-	0183	CLDP	0247	0	0311	3	0375	R---
0058	STOP	0121	K_	0184	STOP	0248	7	0312	=	0376	4---
0059	PRNT	0122	9	0185	=	0249	9	0313	1	0377	3
0060	=	0123	-	0186	R---	0250	6	0314	4	0378	1
0061	K_	0124	1	0187	R---	0251	=	0315	1	0379	-
0062	9	0125	)	0188	0	0252	R---	0316	5	0380	2
				0189	0	0253	4---	0317	9	0381	)

FIGURE 1 - Tektronix-31 program to calculate XRD d-spacings.

0382	IF-0	0446	R---	0510	R---	0574	4	0638	5	0702	0
0383	EXC	0447	4---	0511	4---	0575	5	0639	0	0703	0
0384	SUM1	0448	3	0512	3	0576	0	0640	/	0704	0
0385	CONT	0449	1	0513	4	0577	EXC	0641	R---	0705	0
0386	EXC	0450	R---	0514	-	0578	SIN	0642	4---	0706	1
0387	Q	0451	4---	0515	1	0579	LBL	0643	5	0707	=
0388	LBL	0452	3	0516	)	0580	3	0644	2	0708	R---
0389	SUM1	0453	2	0517	IF=0	0581	R---	0645	=	0709	4---
0390	2	0454	+	0518	EXC	0582	4---	0646	R---	0710	7
0391	=	0455	6	0519	COS	0583	5	0647	4---	0711	4
0392	R---	0456	=	0520	CONT	0584	3	0648	5	0712	EXC
0393	R---	0457	R	0521	EXC	0585	+	0649	0	0713	K
0394	3---	0458	4	0522	SIN	0586	1	0650	EXC	0714	CONT
0395	6	0459	3	0523	LBL	0587	=	0651	6	0715	CLDP
0396	5	0460	2	0524	COS	0588	R---	0652	LBL	0716	1
0397	EXC	0461	R---	0525	R---	0589	4---	0653	6	0717	8
0398	TAN	0462	4---	0526	R---	0590	5	0654	R---	0718	0
0399	LBL	0463	3	0527	4---	0591	3	0655	4---	0719	/
0400	Q	0464	3	0528	3	0592	R---	0656	5	0720	R---
0401	R---	0465	+	0529	5	0593	4---	0657	1	0721	4---
0402	R---	0466	6	0530	-	0594	5	0658	/	0722	7
0403	4	0467	=	0531	1	0595	1	0659	R---	0723	2
0404	3	0468	R---	0532	)	0596	+	0660	4---	0724	=
0405	1	0469	4---	0533	IF=0	0597	(	0661	5	0725	R---
0406	-	0470	3	0534	EXC	0598	R---	0662	3	0726	4---
0407	1	0471	3	0535	3	0599	R---	0663	=	0727	7
0408	)	0472	R---	0536	CONT	0600	4---	0664	R---	0728	4
0409	IF=0	0473	4---	0537	EXC	0601	3	0665	4---	0729	PRNT
0410	EXC	0474	3	0538	2	0602	2	0666	5	0730	EXC
0411	SUM0	0475	4	0539	LBL	0603	+	0667	1	0731	K
0412	CONT	0476	+	0540	2	0604	R---	0668	R---	0732	LBL
0413	EXC	0477	6	0541	R---	0605	R---	0669	4---	0733	K
0414	TAN	0478	=	0542	4---	0606	4---	0670	5	0734	PAPR
0415	LBL	0479	R---	0543	5	0607	3	0671	1	0735	PAPR
0416	SUM0	0480	4---	0544	2	0608	3	0672	-	0736	PAPR
0417	1	0481	3	0545	+	0609	)	0673	R---	0737	L
0418	=	0482	4	0546	1	0610	/	0674	4---	0738	O
0419	R---	0483	R---	0547	=	0611	2	0675	5	0739	G
0420	R---	0484	4---	0548	R---	0612	=	0676	0	0740	
0421	3---	0485	3	0549	4---	0613	R---	0677	=	0741	
0422	6	0486	5	0550	5	0614	4---	0678	R---	0742	
0423	5	0487	+	0551	2	0615	5	0679	4---	0743	
0424	EXC	0488	6	0552	R---	0616	1	0680	7	0744	
0425	TAN	0489	=	0553	4---	0617	EXC	0681	2	0745	
0426	LBL	0490	R---	0554	5	0618	SIN	0682	CLDP	0746	
0427	SIN	0491	4---	0555	0	0619	LBL	0683	=	0747	D
0428	R---	0492	3	0556	+	0620	4	0684	K	0748	A
0429	3---	0493	5	0557	(	0621	R---	0685	2	0749	T
0430	6	0494	R---	0558	R---	0622	0	0686	C	0750	E
0431	5	0495	4---	0559	R---	0623	0	0687	O	0751	PAPR
0432	+	0496	3	0560	4---	0624	0	0688	R	0752	PAPR
0433	1	0497	6	0561	3	0625	+	0689	R	0753	PAPR
0434	=	0498	+	0562	1	0626	1	0690	=	0754	PAPR
0435	R---	0499	6	0563	+	0627	=	0691	=	0755	PAPR
0436	3---	0500	=	0564	R---	0628	R---	0692	R---	0756	D
0437	6	0501	R---	0565	R---	0629	0---	0693	4---	0757	
0438	5	0502	4---	0566	4---	0630	0	0694	5	0758	S
0439	R---	0503	3	0567	3	0631	0	0695	3	0759	P
0440	4---	0504	6	0568	2	0632	R AD	0696	-	0760	C
0441	3	0505	EXC	0569	)	0633	GODP	0697	0	0761	
0442	1	0506	1	0570	/	0634	LBL	0698	)	0762	2
0443	+	0507	LBL	0571	2	0635	5	0699	IF=0	0763	T
0444	6	0508	TAN	0572	=	0636	R---	0700	1	0764	H
0445	=	0509	R---	0573	R---	0637	4---	0701	=	0765	E

FIGURE 1 - (continued)

0766	T	0827	R---	0888	0	0949	X+A	1010	PI	1071	=
0767	A	0828	4---	0889	=	0950	9	1011	R---	1072	R---
0768		0829	7	0890	R---	0951	=	1012	4---	1073	4---
0769	I	0830	4	0891	4---	0952	R---	1013	6	1074	3
0770	N	0831	/	0892	6	0953	4---	1014	4	1075	6
0771	T	0832	2	0893	2	0954	6	1015	/	1076	R---
0772	PAPR	0833	)	0894	R---	0955	3	1016	(	1077	3---
0773	PAPR	0834	=	0895	4---	0956	R---	1017	2	1078	6
0774	PAPR	0835	R---	0896	4	0957	R---	1018	*	1079	5
0775	CLDP	0836	4---	0897	1	0958	3---	1019	R---	1080	+
0776	2	0837	6	0898	*	0959	6	1020	4---	1081	1
0777	=	0838	0	0899	R---	0960	5	1021	6	1082	=
0778	R---	0839	R---	0900	4---	0961	-	1022	3	1083	R---
0779	4---	0840	4---	0901	6	0962	1	1023	)	1084	3---
0780	3	0841	3	0902	1	0963	)	1024	=	1085	6
0781	2	0842	2	0903	+	0964	IF=0	1025	R---	1086	5
0782	CLDP	0843	+	0904	R---	0965	R---	1026	4---	1087	EXC-
0783	3	0844	6	0905	4---	0966	4---	1027	6	1088	8
0784	6	0845	=	0906	4	0967	4	1028	5		
0785	5	0846	R---	0907	2	0968	7	1029	EXC		
0786	=	0847	4---	0908	*	0969	=	1030	B		
0787	R---	0848	3	0909	R---	0970	R---	1031	LBL		
0788	3---	0849	2	0910	4---	0971	4---	1032	B		
0789	6	0850	EXC-	0911	6	0972	6	1033	K-		
0790	5	0851	LN-	0912	1	0973	4	1034	2-		
0791	CLDP	0852	LBL-	0913	X+A	0974	EXC-	1035	-		
0792	6	0853	LN-	0914	3	0975	PI	1036	K-		
0793	=	0854	(	0915	+	0976	CONT	1037	9-		
0794	R---	0855	R---	0916	R---	0977	R---	1038	)		
0795	4---	0856	4---	0917	4---	0978	R---	1039	IF=0		
0796	3	0857	6	0918	4	0979	3---	1040	STOP		
0797	6	0858	0	0919	3	0980	6	1041	CONT		
0798	EXC-	0859	/	0920	*	0981	5	1042	R---		
0799	8	0860	5	0921	R---	0982	-	1043	4---		
0800	LBL-	0861	7	0922	4---	0983	2	1044	6		
0801	8	0862	=	0923	6	0984	)	1045	5		
0802	R---	0863	2	0924	1	0985	IF=0	1046	PRNT		
0803	4---	0864	9	0925	X+A	0986	R---	1047			
0804	4	0865	5	0926	5	0987	4---	1048			
0805	3	0866	8	0927	+	0988	4	1049	R---		
0806	2	0867	)	0928	R---	0989	8	1050	4---		
0807	-	0868	*	0929	4---	0990	=	1051	6		
0808	R---	0869	(	0930	4	0991	R---	1052	2		
0809	4---	0870	2	0931	4	0992	4---	1053	PRNT		
0810	5	0871	/	0932	*	0993	6	1054			
0811	0	0872	R---	0933	R---	0994	4	1055			
0812	=	0873	4---	0934	4---	0995	EXC-	1056	R---		
0813	R---	0874	4	0935	6	0996	PI	1057	R---		
0814	4---	0875	6	0936	1	0997	CONT	1058	4---		
0815	7	0876	)	0937	X+A	0998	R---	1059	3		
0816	6	0877	=	0938	7	0999	4---	1060	6		
0817	EXC-	0878	R---	0939	+	1000	4	1061	PRNT		
0818	9	0879	4---	0940	R---	1001	0	1062			
0819	LBL-	0880	6	0941	4---	1002	=	1063			
0820	9	0881	1	0942	4	1003	R---	1064	3SM2		
0821	R---	0882	CLDP	0943	5	1004	4---	1065	R---		
0822	4---	0883	2	0944	*	1005	6	1066	4---		
0823	7	0884	*	0945	R---	1006	4	1067	3		
0824	6	0885	R---	0946	4---	1007	EXC-	1068	6		
0825	*	0886	4---	0947	6	1008	PI	1069	+		
0826	(	0887	6	0948	1	1009	LBL-	1070	6		

FIGURE 1 - (continued)

FIGURE 2 - A simplified version of the complete flow chart.

FIGURE 3A - Flow chart for program (Sec. A).

B

FIGURE 3B - Flow chart for program (Sec. B).

FIGURE 3C - Flow chart for program (Sec. C).

D

FIGURE 3D - Flow chart for program (Sec. D).

which is used to determine whether the data calculated is based on copper $K\alpha$, $K\alpha_1$, or $K\alpha_2$ radiation. There are 30 more R_{---} registers reserved for decision making and constant value storage. Since the data computed is immediately printed and not stored, an excess of 150-plus storage registers remain for the expansion of the program.

The line measurements are collected in the usual manner. The program begins by typing out the label and then asks the user for the number of sets of data to be entered N, followed by an equal sign (=). The user answers the question by striking the appropriate numeral/s key, for example, 37. Depressing the continue (CONT) button causes the paper to advance and the calculator to respond with a typed symbol for the left line measurement, for example, L (I). Each user input is preceded by a symbol: left line L(I), middle line M(I), right line R(I). See Figure 4. A one (1) entered after C(I) indicates that the data in that input set will be used in computing the film correction factor. A one (1) following B(I) indicates that the line is a back reflection line. A one (1) entered after L(I) indicates the line to be a $K\alpha$ line. A two (2) following L(I) indicates the line is a $K\alpha_2$. A value greater than 2, or a zero (0) entered after L(I) indicates the line is a $K\alpha$ (av). Values entered after I(I) are the observed intensities of each line and are based on a scale from 10 to 1 with 10 being the most intense and 1 indicating the line is barely visible.

When all of the line measurements and symbols (for example, 0, 1, and 2) have been entered, the data are completed and printed line by line. The printed data from a typical powder pattern are shown in Figures 5a and 5b. The paper tape output serves as a permanent record for the user.

Program to CALC
D Spacings
Enter N=10

L(I)	76.3	R(I)	0.	B(I)	0.
M(I)	151.	C(I)	0.	I(I)	1.
R(I)	0.	B(I)	0.	L(I)	0.
C(I)	1.	I(I)	2.	M(I)	225.2
B(I)	0.	L(I)	0.	R(I)	362.9
I(I)	9.	M(I)	193.3	C(I)	1.
L(I)	70.2	R(I)	0.	B(I)	1.
M(I)	157.	C(I)	0.	I(I)	2.
R(I)	0.	B(I)	0.	L(I)	0.
C(I)	1.	I(I)	1.	M(I)	243.5
B(I)	0.	L(I)	0.	R(I)	344.7
I(I)	10.	M(I)	209.	C(I)	1.
L(I)	50.7	R(I)	0.	B(I)	1.
M(I)	176.7	C(I)	0.	I(I)	2.
R(I)	0.	B(I)	0.	L(I)	0.
C(I)	1.	I(I)	1.	M(I)	261.2
B(I)	0.	L(I)	0.	R(I)	327.1
I(I)	6.	M(I)	220.9	C(I)	1.
L(I)	0.	R(I)	0.	B(I)	1.
M(I)	189.3	C(I)	0.	I(I)	1.

FIGURE 4 - Sample input data for Tektronix-31 d-spacing program.

Corr.=
.9975062344
Log Date
D_Spc 2Theta Int

2.413332908	62.89276808	1.	111.2718204
37.25685786	6.	1.043792781	2.
9.	1.259725815	95.11221945	.8522337398
2.092168702	75.46134663	1.	129.5261845
43.24189526	2.	.9583072861	2.
10.	1.205194215	106.9825436	.8036222561
1.477648404	79.45137157	1.	147.1820449
		.9338830885	1.

FIGURE 5a - Output data from program used to process d-spacings when a camera radius correction is computed (that is, when back reflection lines are available).

Corr.=
1.0000
Log Date
D_Spc 2Theta Int

2.321981695#	1.564694702#
38.78#	58.98#
1.#	6.#
2.255012374#	1.480930355#
39.98#	62.68#
4.#	4.#
2.186952114#	1.285711174#
41.28#	73.68#
8.#	3.#
2.156998153#	1.25804294#
41.88#	75.58#
10.#	3.#
2.095609181#	1.212198652#
43.13#	78.98#
7.#	3.#

FIGURE 5b - Output data from program used to process d-spacings when no back reflection lines are available (that is, when the camera radius correction equals 1.000).

Conclusions

The program described in this report represents the initial attempt by the X-ray diffraction laboratory personnel to provide X-ray data computation backup to the PDP-8/I computer. The Tektronix-31 calculator has shown that it is an

accurate, relatively rapid, and satisfactory tool - able to provide the necessary data computations in the event of a temporary loss of the PDP-8/I computer services.

Glossary of Program Terms

N Number of lines read from X-ray powder diffraction pattern.

PI 3.14159

SL Sum left, which is

$$SL + \sum_{l=1}^k \left(\frac{\text{left} + \text{middle}}{2} \right)$$

SR Sum right, which is

$$SR + \sum_{l=1}^l \left(\frac{\text{middle} + \text{right}}{2} \right)$$

Left = lines which are located to the left of the hole at the left side of the film punched for standard Wilson or Strausman's load cameras.

Middle = lines which are located between the left and right holes on the film.

Right = lines located to the right of the hole at the right side of the film.

L Counter used to determine SL average.

R Counter used to determine SR average.

Corr. Camera correction factor which adjusts data for film expansion or shrinkage.

DELTA Middle line minus SL average.

Subroutines Used

1)	DG/R	11)	3
2)	1	12)	5
3)	SIN	13)	6
4)	HYP	14)	K
5)	SUM 0	15)	8
6)	SUM 1	16)	9
7)	Q	17)	LN
8)	TAN	18)	PI
9)	COS	19)	B
10)	2		

NOTE: All subroutines are appropriately labeled and defined on the flow chart which appears in Figure 2.

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1. P. W. Seabaugh and R. R. Eckstein, Program for Calculating X-Ray Diffraction Interplanar (d) Spacings with a PDP-8/I Computer, MLM-1646 (Oct. 15, 1969).
2. Tektronix-31 Operators Manual, Tektronix, Inc., Beaverton, Oregon (1973).

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