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STRUCTURE DETERMINATION I

by

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STRUCTURE DETERMINATION I

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A program, called Structure I, to calculate the structure factor or intensity for a given set of reflections is written in Bell language for the IBM 650. Each $\sin^2 \theta$, multiplicity and scattering factor for each element must be entered. The program has space for a maximum of 100 atomic positions and 18 elements. Roughly about 10 seconds is needed per reflection.

The data must be entered in floating decimal point arithmetic and the answers will also be in this system. In this system the last two digits indicate the position of the decimal point. For example,

1000000050 denotes 1×10^0 or 1
 1000000049 denotes 1×10^{-1} or 0.1
 1000000052 denotes 1×10^2 or 100 .

Either the structure factor or the intensity may be calculated. The appropriate Lorentz-polarization correction may be chosen from the several listed in the program. The Lorentz correction is also entered alone. The program also contains the option of using a temperature correction, absorption correction, or dispersion correction. There is provision for entering either the observed structure factors or intensities and calculating ΔF or ΔI , and summing ΔF or ΔI . There is also provision for printing $\sum f \cos (hx + ky + lz)$ and $\sum f \sin (hx + ky + lz)$ for each element.

These are the various formulas used in the program with the register in which the calculation is begun.

Register 415 - Structure factor

$$A = \sum f \cos (hx + ky + lz)$$

$$B = \sum f \sin (hx + ky + lz)$$

$$F^2 = A^2 + B^2$$

Register 577 - Intensity $I = F^2 LP p T A$

Register 582 - ΔF or ΔI $F_c - F_0 = \Delta F$; $\sum \Delta F$ in register 080

Temperature correction - Register 559

$$T = e^{-B (\sin^2 \theta / \lambda^2)}$$

Register 468 - Dispersion correction

$$f = f_0 + \Delta f' + \frac{(\Delta f'')^2}{2(f_0 + \Delta f')}$$

where f_0 is the normal function of $\sin \theta/\lambda$; f' , f'' given in Acta Cryst. 8:841 (1955).

Register 461 - Lorentz correction

$$L = \frac{1}{\sin 2\theta \sin \theta} = \frac{1}{2 \sin^2 \theta \cos \theta}$$

Register 551 - Lorentz-polarization correction for powder photographs

$$LP = \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}$$

Register 404 - Lorentz-polarization correction for the zero layer line of single crystal rotation or Weissenberg photographs.

$$LP_{II} = \frac{1 + \cos^2 2\theta}{\sin 2\theta} = \frac{1 + \cos^2 2\theta}{2 \sin \theta \cos \theta}$$

Register 564 - Lorentz-polarization correction for rotation and normal incidence Weissenberg photographs. (α is the angle between the axis of rotation and the reflecting planes,)

$$LP_{III} = \frac{1 + \cos^2 2\theta}{\sin 2\theta} \frac{\cos \theta}{(\cos^2 \alpha - \sin^2 \theta)^{1/2}} = \frac{1 + \cos^2 2\theta}{2 \sin \theta \cos \theta} \frac{\cos \theta}{(\cos^2 \alpha - \sin^2 \theta)^{1/2}} = \frac{1 + \cos^2 2\theta}{2 \sin \theta (\cos^2 \alpha - \sin^2 \theta)^{1/2}}$$

The absorption correction goes in register 061. There is space in the program in registers 650-699 to calculate the absorption correction for each reflection.

PREPARATION OF DATA CARDS

The atomic coordinates are listed in order in a block of registers, i.e., x's in 101, etc.; y's in 201, etc.; and z's in 301, etc. The atomic coordinates must be given in degrees in floating decimal point arithmetic. Place the register number in col. 7-9, words per card in col. 10, sign and angle in following columns and program number in col. 77-79. For each card in a series add the number of words on the previous card to the number in col. 7-9.

Prepare the reflection cards as follows. The register number of the first card is 700. Add the words per card to the register number to get the register number for the following card. Use as many cards as necessary for each reflection. It is suggested that the cards be numbered consecutively in the col. 77-79 so that they can easily be kept in order.

<u>Location</u>	<u>Contents</u>	<u>Description</u>
700	+ 0 00h 00k 00l	hkl
701	+ X XXX XXX XXX	$\sin^2 \theta$
702	sign h 000 000 050	(Use floating point arithmetic)
703	sign k 000 000 050	
704	sign l 000 000 050	
705	+ X XXX XXX XXX	Multiplicity (If not used, this must be filled with +1 000 000 005)
706	+ X XXX XXX XXX	Scattering factor for first element in floating point arithmetic
7XX	+ X XXX XXX XXX	Ditto for second element, etc., until all elements are listed.

If the temperature correction is to be used, put B in register 060. If the absorption correction is desired, it goes in 061. To tabulate $\Sigma \Delta F$ or $\Sigma \Delta I$, put the observed intensities or structure factors in the same order as the reflection cards starting in register 740-799. To calculate LP_{III} , put the wavelength of radiation used in register 057 and the angle between the axis of rotation and reflecting planes in register 055. To calculate the dispersion correction, prepare the following cards:

<u>Location</u>	<u>Contents</u>	<u>Description</u>
900	X XXX XXX XXX	f'' for the first element
901	X XXX XXX XXX	f' for the first element
902	X XXX XXX XXX	f'' for the second element
903	X XXX XXX XXX	f' for the second element, etc.

The instruction cards set up the program for the individual problem. Some instructions are mandatory in every problem and some are optional. The optional instructions may be omitted if the particular calculation is not to be performed.

MANDATORY INSTRUCTION CARDS

<u>Location</u>	<u>Contents</u>	<u>Description</u>
600	+ 0 005 591 XXX	100 + number of atomic coordinates
601	+ 0 005 592 XXX	200 + number of atomic coordinates
602	+ 0 005 593 XXX	300 + number of atomic coordinates

<u>Location</u>	<u>Contents</u>	<u>Description</u>
603	+ 0 006 402 XXX	000 + number of elements
604	+ 0 050 449 XXX	000 + number of elements
605	+ 0 060 435 XXX	000 + number of elements
606	+ 0 050 427 XXX	000 + number of atomic positions for the first element
607	+ 0 005 439 XXX	000 + number of atomic positions for the first element
608	+ 0 005 500 XXX	000 + number of atomic positions for the second element
609	+ 0 005 503 XXX	000 + number of atomic positions for the third element, etc. Add 3 to the B address (500) for each additional element. You are lim- ited to 18 elements.
6XX	+ 0 203 000 590	The last instruction of the set.

OPTIONAL INSTRUCTIONS

Instructions to Calculate Intensity

6XX	+ 0 005 403 XXX	*Type of Lorentz-polarization cor- rection to be used. Powder - 551. Single Crystal, zero layer, - 404. Single Crystal, multiple layer, - 564
6XX	+ 0 005 403 461	*To use Lorentz correction only
6XX	+ 0 005 456 XXX	*To use Temperature correction, - 559. Without Temperature correc- tion - 577.

Instructions to Calculate Dispersion

6XX	+ 0 005 403 468	Transfer to dispersion calculation
6XX	+ 0 050 481 XXX	000 + number of elements
6XX	+ 0 005 489 XXX	Transfer to correct type of calcula- tion. Structure factor - 415. LP (powder) - 551. LP (zero layer) - 404. LP (multiple layer) - 564. Lorentz - 461

*Only one instruction with the same B address can be used per program.

<u>Location</u>	<u>Contents</u>	<u>Description</u>
To $\Sigma\Delta F$ or $\Sigma\Delta I$		
6XX	+ 0 005 581 582	
6XX	+ 0 500 582 703	If want $\Sigma\Delta I$ instead of $\Sigma\Delta F$
6XX	+ 0 005 456 582	*If want $\Sigma\Delta F$ and I is not calculated
6XX	+ 0 006 582 XXX	If want f's printed, 000 + 2 x number of elements
6XX	+ 0 005 563 582	If Temperature correction is used and intensity is not calculated
To control size of print out		
6XX	+ 0 006 458 XXX	000 + number of items beyond F which you want printed
6XX	+ 0 600 457 XXX	000 + number of items beyond F which you want printed

In both programs the 603 instruction must include all the elements on the 700 series cards. The 604 and 605 instructions can include only the first one or two elements if the heavier elements are to be adjusted before including the lighter elements.

In cases where a number of atomic coordinate positions could be re-written as $n_f [\cos (hx + ky + lz) + \sin (hx + ky + lz)]$, the computing time and the amount of input data can be shortened by multiplying the scattering curve for the element before entry or have the machine do this in registers 012-049. The number 2 is in register 400, but the other numbers would have to be placed in empty registers in floating point arithmetic. These instructions would have to be entered.

<u>Location</u>	<u>Contents</u>	<u>Description</u>
6XX	+ 0 005 403 020	*Transfer instruction
020	+ 3 706 XXX 706	Register containing scattering curve times register containing the multiplier
021	+ 3 707 XXX 707	Register containing scattering curve times register containing the multiplier
02X	+ 0 203 000 XXX	Last instruction; transfer to type of calculation. Structure factor - 415. LP (powder) - 551. LP (zero layer) - 404. LP (multiple layer) - 564. Lorentz - 461.

*Only one instruction with the same B address can be used per program.

If the dispersion is to be calculated, this should be calculated first and then the scattering factor changed; in other words, the instructions should be as follows:

<u>Location</u>	<u>Contents</u>	<u>Description</u>
6XX	+ 0 005 403 468	*Transfer to calculate dispersion
6XX	+ 0 005 489 020	Transfer to increase scattering factor

RESULTS

The results of the calculations will be printed out in the following manner. First, the atomic coordinates on which the calculations were based will be printed out; all the x's in the 100's, y's in 200's and z's in 300's. Then the calculation for the individual reflections will be listed.

<u>Location</u>	<u>Contents</u>
700	hkl
701	$\sin^2 \theta$
702	F
703	I
704	$\Sigma f \cos (hx + ky + lz)$ for the first element
705	$\Sigma f \sin (hx + ky + lz)$ for the first element
706	$\Sigma f \cos (hx + ky + lz)$ for the second element, etc.
7XX	ΔF or ΔI

INSTRUCTIONS FOR RUNNING THE PROGRAM

The cards must be loaded in the read hopper of the 533 (read-punch unit of the IBM 650) face down, 12 edge down (top towards the back of the machine) as follows.

Bell Deck
 Program deck
 600 series data cards
 055 containing α (optional)
 056 containing B (optional)
 057 containing wavelength (optional)
 061 containing A (optional)
 740-799 containing F_0 or I_0 (optional)
 Atomic coordinate cards
 Transfer card 600
 Reflection cards
 5 blank cards

Blank cards are placed in the punch hopper of the 533 face down, 12 edge down. The Bell control board (9) is placed in the 533.

The controls on the console are set:

Storage Entry	70 1951 1333 +
Programmed Stop	Stop
Half Cycle	Run
Address Selection	XXXX
Control	Run
Display	Upper Accumulator
Overflow	Stop
Error	Stop

Depress the following keys in the following order:

Computer Reset
 Program Start
 Start (on card reader)
 Depress start on the punch side of the card reader

If it is desired to run a series of different angles with the same reflection cards at the end of the first run, remove the cards from the read hopper, place the new atomic coordinate cards, transfer card for 590, the reflection cards and the five blank cards in the read unit, and depress the keys as before.

To obtain the $\Sigma \Delta F$ or $\Sigma \Delta I$ at the end of the run, place the 080 transfer card in the read unit and depress the keys as before. The answer will appear in 080 on one card.

The answer cards are placed in the 407 (tabulator unit) face down, 9 edge down (top to front of machine). The Bell board (77) is placed in the 407. The start button is pushed and your cards are listed.

STRUCTURE II

This program for Structure II is the same as Structure I except for the instructions between 415-460 and 500-550. It allows one to calculate either cos or sin alone with some saving of time over that of Structure I. All the various data cards, reflection cards, etc., except the 600 series of instruction cards, are the same as in Structure I. The operating directions are the same and the print out will be the same except only that $\Sigma f \cos (hx + ky + lz)$ or $\Sigma f \sin (hx + ky + lz)$ is given.

MANDATORY INSTRUCTION CARDS

<u>Location</u>	<u>Contents</u>	<u>Description</u>
600	+ 0 005 591 XXX	100 + number of atomic coordinates
601	+ 0 005 592 XXX	200 + number of atomic coordinates
602	+ 0 005 593 XXX	300 + number of atomic coordinates
603	+ 0 006 402 XXX	000 + number of elements
604	+ 0 060 430 XXX	000 + number of elements
605	+ 0 050 441 XXX	000 + number of elements
606	+ 0 050 425 XXX	000 + number of atomic coordinates for first element
607	+ 0 050 434 XXX	000 + number of atomic coordinates for first element
608	+ 0 005 500 XXX	000 + number of atomic coordinates for second element. Add 3 to the B address (500) for each additional element
6XX	+ 0 203 000 590	The last instruction in the set

OPTIONAL INSTRUCTIONS

Instructions to calculate intensity

6XX	+ 0 005 403 XXX	*Type of Lorentz-polarization correction to be used. Powder - 551. Single Crystal, zero layer, - 404. Single Crystal, multiple layer, - 564
6XX	+ 0 005 403 461	*To use Lorentz correction only
6XX	+ 0 005 444 XXX	*To use Temperature correction - 559 Without Temperature correction - 577

Instructions to calculate dispersion

6XX	+ 0 005 403 468	
6XX	+ 0 050 481 XXX	000 + number of elements
6XX	+ 0 005 486 XXX	To correct type of calculation. Structure factor - 415. LP _I (powder) - 551. LP _{II} (zero layer) - 404. LP _{III} (multiple layer) - 564. Lorentz - 461

*Only one instruction with the same B address can be used per program.

<u>Location</u>	<u>Contents</u>	<u>Description</u>
To $\Sigma\Delta F$ or $\Sigma\Delta I$		
6XX	+ 0 005 581 582	
6XX	+ 0 500 582 703	If want $\Sigma\Delta I$ instead of $\Sigma\Delta F$
6XX	+ 0 005 444 582	*If want $\Sigma\Delta F$ and I is not calculated
6XX	+ 0 006 582 XXX	If want f's printed, 000 + number of elements
6XX	+ 0 005 563 582	If the temperature correction is used and the intensity is not calculated
To calculate sin instead of cos		
6XX	+ 0 500 420 353	
To control size of print out		
6XX	+ 0 006 458 XXX	000 + number of items beyond F which you want printed
6XX	+ 0 600 457 XXX	000 + number of items beyond F which you want printed

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Dauben, Carol H., and Templeton, David H., Table of Dispersions Corrections for X-ray Scattering of Atoms, Acta Crys. 8,841 (1955).

James, R. W., The Optical Principles of the Diffraction of X-rays, G. Bell and Sons Ltd., London (1948).

*Only one instruction with the same B address can be used per program.

PROGRAM FOR STRUCTURE II
(All instructions are positive)

<u>Location</u>	<u>Contents</u>	<u>Description</u>
060	1 000 000 050	
061	1 000 000 050	
080	0 410 080 081	Punch
400	2 000 000 050	
401	1 000 000 050	
402	0 400 700 705	Read in reflection cards
403	0 203 000 415	Transfer to calculate F only
404	2 401 701 008	$1 - \sin^2 \theta = \cos^2 \theta$
405	0 300 000 002	$\cos \theta$
406	2 008 701 000	$\cos^2 \theta - \sin^2 \theta = \cos 2 \theta$
407	3 000 000 000	$\cos^2 2 \theta$
408	1 000 401 009	$1 + \cos^2 2 \theta$
409	0 300 701 000	$\sin \theta$
410	4 009 000 000	$\div \sin \theta$
411	4 000 002 000	$\div \cos \theta$
412	4 000 400 004	$\div 2 =$ polarization for single crystal Weissenberg
413	0 203 000 415	Transfer to calculate intensity
415	3 702 101 005	hx
416	3 703 201 006	ky
417	3 704 301 000	lz
418	1 000 006 000	ky + lz
419	1 000 005 007	hx + ky + lz
420	0 354 000 000	$\cos (hx + ky + lz)$
421	1 000 050 050	$\Sigma \cos$
422	0 353 007 000	$\sin (hx + ky + lz)$
423	1 000 051 051	$\Sigma \sin$
424	0 060 415 001	
425	0 060 416 001	
426	0 060 417 001	
427	0 100 XXX 415	Loop
428	3 706 050 800	$f_1 \cos$
429	3 706 051 801	$f_1 \sin$
430	9 002 010 050	Clear registers to zero
431	0 600 428 001	Set up for next element
432	0 600 429 001	
433	0 006 428 002	
434	0 006 429 002	
435	6 428 706 500	Test to determine if all the elements have been used

Location	Contents	Description
436	0 050 415 101	Initialize
437	0 050 416 201	Initialize
438	0 050 417 301	Initialize
439	0 050 427 XXX	Initialize set loop for number of atomic coordinates for the first element
440	0 005 435 500	Initialize
441	0 500 428 706	Initialize
442	0 500 429 706	Initialize
443	0 005 428 800	Initialize
444	0 005 429 801	Initialize
445	1 800 980 980	$\Sigma F \cos$
446	1 801 981 981	$\Sigma F \sin$
447	0 600 445 002	
448	0 600 446 002	
449	0 100 XXX 445	Loop
450	0 500 445 800	Initialize
451	0 500 446 801	Initialize
452	3 980 980 499	$F^2 \cos$
453	3 981 981 000	$F^2 \sin$
454	1 000 499 498	F^2
455	0 300 000 702	F
456	0 203 000 457	Transfer to punch F
457	9 000 800 704	Move small f's
458	0 410 700 702	Punch results
459	9 002 010 980	Clear
460	0 203 000 402	Calculate next reflection
461	2 401 701 000	$1 - \sin^2 \theta = \cos^2 \theta$
462	0 300 000 008	$\cos \theta$
463	0 203 000 464	
464	4 401 701 000	$1 \div \sin^2 \theta$
465	4 000 008 000	$\div \cos \theta$
466	4 000 400 004	$\div 2 = \text{Lorentz correction}$
467	0 203 000 415	
468	1 706 901 000	$f_0 + \Delta f'$
469	3 000 400 015	$2(f_0 + \Delta f')$
470	3 900 900 000	$(\Delta f'')^2$
471	4 000 015 000	$(\Delta f'')^2 / 2(f_0 + \Delta f')$
472	1 000 901 000	$f' + (\Delta f'')^2 / 2(f_0 + \Delta f')$
473	1 000 706 706	$f_0 + f' + (\Delta f'')^2 / 2(f_0 + \Delta f')$
474	0 600 468 001	
475	0 060 468 002	

<u>Location</u>	<u>Contents</u>	<u>Description</u>
476	0 600 470 002	
477	0 060 470 002	
478	0 060 472 002	
479	0 060 473 001	
480	0 006 473 001	
481	0 100 000 468	Loop
482	0 500 468 706	Initialize
483	0 050 468 901	Initialize
484	0 500 470 900	Initialize
485	0 050 470 900	Initialize
486	0 050 472 901	Initialize
487	0 050 473 706	Initialize
488	0 005 473 706	Initialize
489	0 203 000 415	Transfer to calculate F
500	0 050 427 XXX	Atomic positions for 2nd element
501	0 005 435 503	
502	0 203 000 415	
503	0 050 427 XXX	Atomic positions for 3rd element
504	0 005 435 506	
505	0 203 000 415	
506	0 050 427 XXX	Atomic positions for 4th element
507	0 005 435 509	
508	0 203 000 415	
509	0 050 427 XXX	Atomic positions for 5th element
510	0 005 435 512	
511	0 203 000 415	
512	0 050 427 XXX	Atomic positions for 6th element
513	0 005 435 515	
514	0 203 000 415	
515	0 050 427 XXX	Atomic positions for 7th element
516	0 005 435 518	
517	0 203 000 415	
518	0 050 427 XXX	Atomic positions for 8th element
519	0 005 435 521	
520	0 203 000 415	
521	0 050 427 XXX	Atomic positions for 9th element
522	0 005 435 524	
523	0 203 000 415	
524	0 050 427 000	Atomic positions for 10th element
525	0 005 435 527	
526	0 203 000 415	
527	0 050 427 000	Atomic positions for 11th element
528	0 005 435 530	

<u>Location</u>	<u>Contents</u>	<u>Description</u>
529	0 203 000 415	Atomic positions for 12th element
530	0 050 427 000	
531	0 005 435 533	
532	0 203 000 415	Atomic positions for 13th element
533	0 050 427 000	
534	0 005 435 536	
535	0 203 000 415	Atomic positions for 14th element
536	0 050 427 000	
537	0 005 435 539	
538	0 203 000 415	Atomic positions for 15th element
539	0 050 427 000	
540	0 005 435 542	
541	0 203 000 415	Atomic positions for 16th element
542	0 050 427 000	
543	0 005 435 545	
544	0 203 000 415	Atomic positions for 17th element
545	0 050 427 000	
546	0 005 435 548	
547	0 203 000 415	Atomic positions for 18th element
548	0 050 427 000	
549	0 005 435 982	
550	0 203 000 415	$1 - \sin^2 \theta = \cos^2 \theta$
551	2 401 701 008	
552	0 300 000 002	
553	2 008 701 000	$\cos \theta$
554	3 000 000 000	$\cos^2 \theta - \sin^2 \theta = \cos 2 \theta$
555	1 000 401 000	$\cos^2 2 \theta$
556	4 000 701 000	$1 + \cos^2 2 \theta$
557	4 000 002 004	$\frac{1}{2} \sin^2 \theta$
558	0 203 000 415	$\frac{1}{2} \cos \theta = \text{polarization for powder}$
559	4 701 057 000	Transfer to calculate F
560	4 000 057 000	$\sin^2 \theta / \lambda$
561	5 000 056 058	$\div \lambda$
562	0 301 058 060	$-B (\sin \theta / \lambda^2)$
563	0 203 000 577	= Temperature correction
564	0 300 701 052	Transfer to calculate intensity
565	2 401 701 008	$\sin \theta$
566	2 008 701 053	$1 - \sin^2 \theta = \cos^2 \theta$
567	3 000 000 054	$\cos^2 \theta - \sin^2 \theta = \cos 2 \theta$
568	1 000 401 009	$\cos^2 2 \theta$
569	0 354 055 000	$1 + \cos^2 2 \theta$
570	3 000 000 000	$\cos \alpha$
571	2 000 701 000	$\cos^2 \alpha$
		$\cos^2 \alpha - \sin^2 \theta$

<u>Location</u>	<u>Contents</u>	<u>Description</u>
572	0 300 000 000	$\sqrt{\cos^2 \alpha - \sin^2 \theta}$
573	4 009 000 000	$1 + \cos^2 2\theta / \sqrt{\cos^2 \alpha - \sin^2 \theta}$
574	4 000 052 000	$\div \sin \theta$
575	4 000 400 004	$\div 2 =$ polarization for upper layer lines on Weissenberg and rotation photographs
576	0 203 000 415	Transfer to calculate F
577	3 498 004 000	F^2LP
578	3 000 705 000	F^2LPp
579	3 000 060 000	F^2LPpT
580	3 000 061 703	$F^2LPpTA = I$
581	0 203 000 457	Transfer to punch results
582	2 702 740 704	$F_c - F_0 = \Delta F$
583	1 000 080 080	$\Sigma \Delta F$
584	0 060 582 001	
585	0 203 000 457	Transfer to punch results
590	0 050 582 740	
591	0 410 101 102	Punch atomic coordinates
592	0 410 201 202	Punch atomic coordinates
593	0 410 301 302	Punch atomic coordinates
594	9 001 010 080	Clear $\Sigma \Delta I$ or $\Sigma \Delta F$
595	0 203 000 402	Calculate next reflection

UNIQUE INSTRUCTIONS FOR STRUCTURE III

<u>Location</u>	<u>Contents</u>	<u>Description</u>
415	3 702 101 005	hx
416	3 703 201 006	ky
417	3 704 301 000	lz
418	1 000 006 000	lz + ky
419	1 000 005 007	hx + ky + lz
420	0 354 000 000	cos (hx + ky + lz)
421	1 000 050 050	cos (hx + ky + lz)
422	0 060 415 001	
423	0 060 416 001	
424	0 060 417 001	
425	0 100 XXX 415	
426	3 706 050 800	$f_1 \cos (hx + ky + lz)$
427	9 001 010 050	Clear to zeros
428	0 600 426 001	
429	0 006 426 001	
430	6 426 706 500	Test if all elements have been calculated
431	0 050 415 101	Initialize
432	0 050 416 201	Initialize
433	0 050 417 301	Initialize
434	0 050 425 XXX	Set first loop
435	0 500 426 706	Set first loop
436	0 005 426 800	Set first loop
437	0 005 430 500	Set first loop
438	9 001 010 702	Clear
439	1 800 702 702	F
440	0 600 439 001	
441	0 100 XXX 439	100 loop
442	0 500 439 800	
443	3 702 702 498	F^2
444	0 203 000 457	Transfer to print
457	9 000 800 704	Move f cos (hx + ky + lz)
458	0 410 700 702	Print
459	0 203 000 402	
500	0 050 425 XXX	Atomic coordinates in second element
501	0 005 430 503	
502	0 203 000 415	
504	0 050 425 XXX	
505	0 005 430 506	
506	0 203 000 415	
507	0 005 430 509	

<u>Location</u>	<u>Contents</u>	<u>Description</u>
508	0 203 000 415	
509	0 050 425 XXX	
510	0 005 430 512	
511	0 203 000 415	
512	0 050 425 XXX	
513	0 005 430 515	
514	0 203 000 415	
515	0 050 425 XXX	
516	0 005 430 518	
517	0 203 000 415	
518	0 050 425 XXX	
519	0 005 430 521	
520	0 203 000 415	
521	0 050 425 XXX	
522	0 005 430 524	
523	0 203 000 415	
524	0 050 425 000	
525	0 005 430 527	
526	0 203 000 415	
527	0 050 425 000	
528	0 005 430 530	
529	0 203 000 415	
530	0 050 425 000	
531	0 005 430 533	
532	0 203 000 415	
533	0 050 425 000	
534	0 005 430 536	
535	0 203 000 415	
536	0 050 425 000	
537	0 005 430 539	
538	0 203 000 415	
539	0 050 425 000	
540	0 005 430 542	
541	0 203 000 415	
542	0 050 425 000	
543	0 005 430 545	
544	0 203 000 415	
545	0 050 425 000	
546	0 005 430 548	
547	0 203 000 415	
548	0 050 425 000	
549	0 005 430 982	
550	0 203 000 415	