15-sequences differs in at most one sign from one of the set of 2048. In the crystallographic application we may say that one member of S must be 'substantially correct', or that S *substantializes* the set of all possible 15-sequences. The use of S saves a work factor of 16 provided that we can stand one wrong sign. The general problem of substantialization remains open.

Denote a typical 15-sequence (an ordered sequence of fifteen signs, or of symbols $+1$ and -1) by $a_1, a_2, a_3, \ldots, a_{15}$, where each a_i is $+1$ or -1. Consider the set, S, of 15-sequences satisfying the relationships

$$\left.\begin{aligned} a_1a_2a_3a_4a_5a_6a_7a_8 &= 1, \\ a_1a_2a_3a_4a_9a_{10}a_{11}a_{12} &= 1, \\ a_1a_2a_5a_6a_9a_{10}a_{13}a_{14} &= 1, \\ a_1a_3a_5a_7a_9a_{11}a_{13}a_{15} &= 1. \end{aligned}\right\} \quad (1)$$

Note first that S has precisely 2048 members; for $a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_9, a_{10}, a_{11}, a_{13}$ can be selected arbitrarily (in 2^{11} ways) and then a_8, a_{12}, a_{14} and a_{15} can be determined uniquely from (1). Now if any pair of symbols is selected from $a_1, a_2, a_3, \ldots, a_{15}$, then one of the four relationships contains one of the pair and not the other, so a change of sign of two symbols in a member of S cannot transform this member into another one. Therefore the 16×2048 15-sequences obtained by taking the 2048 sequences of S, together with the ones obtained by changing one sign in each of them in all possible ways, must be all distinct. And since there are only 16×2048 possible 15-sequences they must each occur exactly once.

The relationships (1) were obtained by first writing down the numbers 1, 2, 3, ..., 15, expressed in the binary scale, into the columns of a four-by-fifteen rectangle, thus:

```
0 0 0 0 0 0 0 1 1 1 1 1 1 1 1
0 0 0 1 1 1 1 0 0 0 0 1 1 1 1
0 1 1 0 0 1 1 0 0 1 1 0 0 1 1
1 0 1 0 1 0 1 0 1 0 1 0 1 0 1,
```

then writing the symbols $a_{15}, a_{14}, a_{13}, \ldots, a_1$ at the tops of the columns (any order would have done just as well), and finally defining one relationship by each *row* of the rectangle using 1's to mean presence and 0's to mean absence. The process can clearly be applied to n-sequences, whenever n is 1 less than a power of 2, and in particular it covers the set presented by Woolfson, with $n = 7$.

The set S could be written down manually by the rule described in the proof that it has 2048 members. By making use of an electronic computer the set S could be used without actually being written down on paper. It is possible that it would sometimes be desirable to combine the use of S with other techniques that are appropriate for electronic computers, such as the one described by Cochran & Douglas (1953).

The general problem, $\gamma(n, r)$, of substantialization of sign sequences is that of finding economical sets of n-sequences such that every possible n-sequence differs from one of the set in at most r signs. The method given above solves the problems $\gamma(2^m-1, 1)$ and provides perfectly economical solutions for these problems. By simply abutting the sequences of k such solutions we can obtain reasonably economical, but not perfectly economical, solutions of $\gamma(2^{m_1}+2^{m_2}+\ldots+2^{m_k}-k, k)$. (This remark generalizes one made in Woolfson's paper.) For example we can obtain tolerable solutions of $\gamma(14, 2)$, $\gamma(21, 3)$, $\gamma(22, 2)$.

The problem of substantialization occurs in an even more general form in the filling up of coupons for 'football pools', a type of gambling that is popular in the United Kingdom. There are then three states (wins, draws and losses) for the components of the n-sequences instead of only two. Further generalizations may be of value in crystallography for crystals that are not centrosymmetrical. For example, if it is adequate to approximate to the phases to the nearest multiple of 60°, then we should be faced with the problem having six states instead of two or three.

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The unit cell of potassium borohydride, KBH_4, at 90° K.

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In connexion with a nuclear magnetic resonance investigation of $NaBH_4$ and KBH_4, X-ray powder photographs of the two salts at 293° K. and 90° K. have been obtained, and lattice constants derived.

For the X-ray photographs copper radiation from a Metrovic generator was used, the specimen being mounted in a low-temperature camera similar to that described by Hume-Rothery (Hume-Rothery & Strawbridge, 1947), with a Unicam cassette of 19 cm. diameter. The low-temperature photographs were obtained by running a stream of liquid oxygen over the sample.

The $NaBH_4$, supplied by Light and Co., was recrystallized once from water below 5° C. and once, in a vacuum-tight vessel, from iso-propylamine previously dried over lithium hydride (Davis, Mason & Stegeman, 1949). Analysis by acid hydrolysis gave the theoretical quantity of hydrogen. The KBH_4, obtained from May and Baker, by a similar analysis gave 96·1% of the hydrogen required by the formula. Samples were packed into Lindemann glass tubes and sealed with picien. Both these operations were performed in a dry-box.

The following lattice constants were obtained. They are in Ångström units and previously published values are added in brackets.

$NaBH_4$ at 293° K.: face-centred cubic, $a = 6{\cdot}157$ (Soldate (1947), $a = 6{\cdot}151 \pm 0{\cdot}009$; Abrahams & Kalnajs (1954), $a = 6{\cdot}1635 \pm 0{\cdot}0005$).

$NaBH_4$ at 90° K.: body-centred tetragonal, $a = 4{\cdot}353$, $c = 5{\cdot}909$ (Abrahams & Kalnajs (1954), $a = 4{\cdot}354 \pm 0{\cdot}005$, $c = 5{\cdot}907 \pm 0{\cdot}005$).
KBH_4 at 293° K.: face-centred cubic, $a = 6{\cdot}722$ (Abrahams & Kalnajs (1954), $a = 6{\cdot}7272 \pm 0{\cdot}0005$).
KBH_4 at 90° K.: face-centred cubic, $a = 6{\cdot}636 \pm 0{\cdot}002$.

The results for $NaBH_4$ and KBH_4 at room temperature, and for $NaBH_4$ at low temperature, are in good agreement with previous measurements (Soldate, 1947; Abrahams & Kalnajs, 1954). Unlike its sodium analogue, KBH_4 at 90° K. shows no change in crystal structure beyond a lattice contraction. Stockmayer & Stephenson (1953) suggested that $NaBH_4$ may change from the cubic form at temperatures below the specific-heat anomaly (Johnston & Hallet, 1953) in order to reduce the repulsive energy between the hydrogen atoms. KBH_4, however, has a more open structure, owing to the larger size of the potassium ion, and remains cubic down to 90° K.

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The unit-cell dimensions of *p*-chlorobenzoic acid.

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In the course of some X-ray investigations on *p*-chlorobenzoic acid, values of the unit-cell dimensions were found differing appreciably from those given by Toussaint (1951).

Seven reflexions chosen for their high Bragg angles from the three principal zones were recorded on a multiple-exposure camera of 14 cm. diameter (Ubbelohde, 1939). Film measurements were made to 0·002 cm. with a travelling microscope, and both α_1 and α_2 reflexions were measured on each film by two independent observers. Calibration was by a platinum substandard against silver ($a = 4{\cdot}0775$ Å) and the radiation employed was Cu $K\alpha$ ($\lambda\alpha_1 = 1{\cdot}5405$ Å, $\lambda\alpha_2 = 1{\cdot}5443$ Å). The planes used, together with their Bragg angles, are given in Table 1.

Table 1. *Planes used*

hkl	$\theta\alpha_1$	$\theta\alpha_2$
13,5,0	75° 20·0′	75° 54·8′
17,$\bar{3}$,0	78° 57·3′	79° 35·3′
870	83° 24·1′	84° 45·3′
9$\bar{7}$0	77° 15·36′	77° 56·73′
12,0,3	68° 32′	68° 56·9′
15,0,$\bar{3}$	75° 51·1′	76° 30·1′
06$\bar{3}$	71° 1·6′	71° 29·3′

The method of least squares was used to find a^*, b^* and γ^* from the ($hk0$) zone, and the remaining reciprocal-lattice parameters were then determined by solving the general equation for the triclinic system:

$$(2 \sin\theta)^2 = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2klb^*c^* \cos\alpha^* + 2lhc^*a^* \cos\beta^* + 2hka^*b^* \cos\gamma^*.$$

These parameters are given in Table 2, together with the unit-cell dimensions derived from them, the figures being

Table 2. *Lattice parameters of p-chlorobenzoic acid at* 18° C.

Reciprocal parameters for $\lambda\alpha_1$		Present work	Deviation from mean	Toussaint
a^*	0·10916 Å^{-1}	a 14·190 Å	±0·004 Å	14·39 Å
b^*	0·24835 Å^{-1}	b 6·213 Å	±0·001 Å	6·29 Å
c^*	0·40158 Å^{-1}	c 3·852 Å	±0·002 Å	3·86 Å
α^*	88° 28′	α 91° 15′	±2′	91° 38′
β^*	84° 36′	β 95° 19′	±1′	95° 18′
γ^*	86° 56′	γ 92° 56′	±1′	92° 44′

the mean of the α_1 and α_2 calculations. The third column shows the deviation from their mean of the values calculated from the α_1 and α_2 observations. The estimated systematic errors are less than these. Toussaint's values are given for comparison.

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