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Symmetry in reciprocal space.

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On account of previous discussions of relations between structure factors by Buerger (1949), MacGillavry (1950), and Waser (1955), the remarks in this paper can be brief. The single objective of this work is to show that the concept of point group can be carried into reciprocal space. In the same manner that each point group in direct space can be represented as (1) a matrix, (2) a set of equivalent positions and (3) a diagram depicting the configuration of equivalent points, reciprocal space presents point groups which can also be represented in these three ways.

Table 1 demonstrates the parallelism between direct and reciprocal space in two dimensions. It is interesting that in representing the point groups in reciprocal space of two dimensions, it is convenient to consider the phase, α, as an added coordinate, as shown in the second to last column of the table. Thus, two-dimensional direct space is associated with three-'dimensional' reciprocal space, hence the symbolism used in the last column to designate the reciprocal-space point groups. The rectangles drawn around the symbols are to prevent confusion with those direct-space symbols in three dimensions that are identical.

Continued investigations have shown that for each of the point groups in three dimensions there are corresponding point groups in four dimensions, (Hermann, 1949; Stuart, 1950), with α as the fourth coordinate of reciprocal space. As has been pointed out by other authors, such considerations are useful in preliminary phase determinations.

References

BUERGER, M. G. (1949). *Proc. Nat. Acad. Sci., Wash.* **35**, 198.

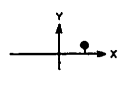
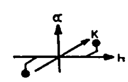
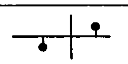
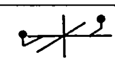
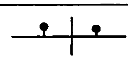
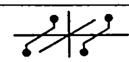
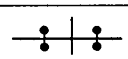
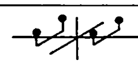
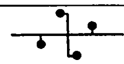
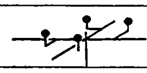
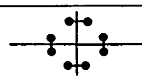
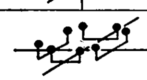
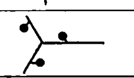
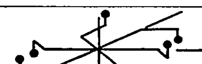
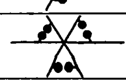
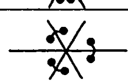
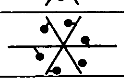
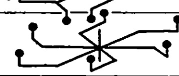
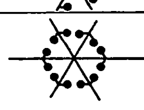
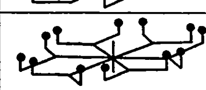
HERMANN, C. (1949). *Acta Cryst.* **2**, 139.

MACGILLAVRY, C. H. (1950). *Acta Cryst.* **3**, 214.

STUART, D. A. (1950). Doctorate Thesis, University of Utah.

WASER, J. (1955). *Acta Cryst.* **8**, 595.

Table 1

DIRECT SPACE				RECIPROCAL SPACE			
Point group	Matrix	Equivalent positions	Configuration	Matrix	Equivalent positions	Configuration	Point group
p1	$\begin{vmatrix}1&0\\0&1\end{vmatrix}$	xy		$\begin{vmatrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&\bar{1}\end{vmatrix}$	$hk\alpha$ $\bar{h}\bar{k}\bar{\alpha}$		$\boxed{\bar{1}}$
p2	$\begin{vmatrix}\bar{1}&0\\0&\bar{1}\end{vmatrix}$	xy $\bar{x}\bar{y}$		$\begin{vmatrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&1\end{vmatrix}$	$hk\alpha$ $\bar{h}\bar{k}\alpha$		$\boxed{2_c}$
pm	$\begin{vmatrix}\bar{1}&0\\0&1\end{vmatrix}$	xy $\bar{x}y$		$\begin{vmatrix}\bar{1}&0&0\\0&1&0\\0&0&1\end{vmatrix}$ & $\begin{vmatrix}1&0&0\\0&\bar{1}&0\\0&0&\bar{1}\end{vmatrix}$	$hk\alpha$ $\bar{h}\bar{k}\bar{\alpha}$ $\bar{h}k\alpha$ $h\bar{k}\bar{\alpha}$		$\boxed{2/m}$
pmm	$\begin{vmatrix}\bar{1}&0\\0&1\end{vmatrix}$ & $\begin{vmatrix}1&0\\0&\bar{1}\end{vmatrix}$	xy $\bar{x}\bar{y}$ $\bar{x}y$ $x\bar{y}$		$\begin{vmatrix}\bar{1}&0&0\\0&1&0\\0&0&1\end{vmatrix}$ & $\begin{vmatrix}1&0&0\\0&\bar{1}&0\\0&0&1\end{vmatrix}$	$hk\alpha$ $\bar{h}\bar{k}\alpha$ $\bar{h}k\alpha$ $h\bar{k}\alpha$		$\boxed{mm}$
p4	$\begin{vmatrix}0&\bar{1}\\1&0\end{vmatrix}$	xy $\bar{x}\bar{y}$ $\bar{y}x$ $y\bar{x}$		$\begin{vmatrix}0&\bar{1}&0\\1&0&0\\0&0&1\end{vmatrix}$	$hk\alpha$ $\bar{h}\bar{k}\alpha$ $k\bar{h}\alpha$ $\bar{k}h\alpha$		$\boxed{4}$
p4m	$\begin{vmatrix}0&\bar{1}\\1&0\end{vmatrix}$ & $\begin{vmatrix}\bar{1}&0\\0&1\end{vmatrix}$	xy $\bar{x}y$ $\bar{x}\bar{y}$ $x\bar{y}$ $y\bar{x}$ $\bar{y}\bar{x}$ $\bar{y}x$ yx		$\begin{vmatrix}0&\bar{1}&0\\1&0&0\\0&0&1\end{vmatrix}$ & $\begin{vmatrix}\bar{1}&0&0\\0&1&0\\0&0&1\end{vmatrix}$	$hk\alpha$ $\bar{h}k\alpha$ $\bar{h}\bar{k}\alpha$ $h\bar{k}\alpha$ $\bar{k}h\alpha$ $\bar{k}\bar{h}\alpha$ $k\bar{h}\alpha$ $kh\alpha$		$\boxed{4m}$
p3	$\begin{vmatrix}0&1\\\bar{1}&\bar{1}\end{vmatrix}$	xy $\bar{y},x-y$ $y-x,\bar{x}$		$\begin{vmatrix}0&1&0\\\bar{1}&\bar{1}&0\\0&0&\bar{1}\end{vmatrix}$	$hk\alpha$ $\bar{h}\bar{k}\bar{\alpha}$ $k,\bar{h}+\bar{k},\alpha$ $\bar{k},h+k,\bar{\alpha}$ $\bar{h}+\bar{k},h,\alpha$ $h+k,\bar{h},\bar{\alpha}$		$\boxed{\bar{3}}$
p3m1	$\begin{vmatrix}0&1\\\bar{1}&\bar{1}\end{vmatrix}$ & $\begin{vmatrix}0&\bar{1}\\\bar{1}&0\end{vmatrix}$	xy $\bar{y}\bar{x}$ $\bar{y},x-y$ $x,x-y$ $y-x,\bar{x}$ $y-x,y$		$\begin{vmatrix}0&1&0\\\bar{1}&\bar{1}&0\\0&0&\bar{1}\end{vmatrix}$ & $\begin{vmatrix}0&\bar{1}&0\\\bar{1}&0&0\\0&0&1\end{vmatrix}$	$\pm$ $hk\alpha$ $\bar{k}\bar{h}\alpha$ $k,\bar{h}+\bar{k},\alpha$ $h+k,\bar{k},\alpha$ $\bar{h}+\bar{k},h,\alpha$ $\bar{h},h+k,\alpha$		$\boxed{\bar{3}2}$
p31m	$\begin{vmatrix}0&1\\\bar{1}&\bar{1}\end{vmatrix}$ & $\begin{vmatrix}0&1\\1&0\end{vmatrix}$	xy yx $\bar{y},x-y$ $\bar{x},y-x$ $y-x,\bar{x}$ $x-y,\bar{y}$		$\begin{vmatrix}0&1&0\\\bar{1}&\bar{1}&0\\0&0&\bar{1}\end{vmatrix}$ & $\begin{vmatrix}0&\bar{1}&0\\\bar{1}&0&0\\0&0&\bar{1}\end{vmatrix}$	$hk\alpha$ $\bar{h}+\bar{k},k,\alpha$ $h+k,\bar{h},\bar{\alpha}$ $k,\bar{h}+\bar{k},\alpha$ $h,\bar{h}+\bar{k},\alpha$ $\bar{k}\bar{h}\bar{\alpha}$ $\bar{h}+\bar{k},h,\alpha$ $\bar{h}\bar{k}\bar{\alpha}$ $h+k,\bar{k},\bar{\alpha}$ $kh\alpha$ $\bar{k},h+k,\bar{\alpha}$ $\bar{h},h+k,\bar{\alpha}$		$\boxed{\bar{3}m1}$
p6	$\begin{vmatrix}0&\bar{1}\\1&1\end{vmatrix}$	xy $\bar{x}\bar{y}$ $\bar{y},x-y$ $y,y-x$ $y-x,\bar{x}$ $x-y,x$		$\begin{vmatrix}0&\bar{1}&0\\1&\bar{1}&0\\0&0&1\end{vmatrix}$	$hk\alpha$ $\bar{h}\bar{k}\alpha$ $k,\bar{h}+\bar{k},\alpha$ $\bar{k},h+k,\alpha$ $\bar{h}+\bar{k},h,\alpha$ $h+k,\bar{h},\alpha$		$\boxed{6}$
p6m	$\begin{vmatrix}0&\bar{1}\\1&1\end{vmatrix}$ & $\begin{vmatrix}\bar{1}&0\\0&\bar{1}\end{vmatrix}$	xy $\bar{x}\bar{y}$ $\bar{y},x-y$ $y,\bar{x}-\bar{y}$ $y-x,\bar{x}$ $\bar{y}-\bar{x},x$ yx $\bar{y}\bar{x}$ $\bar{x},y-x$ $x,\bar{y}-\bar{x}$ $x-y,\bar{y}$ $\bar{x}-\bar{y},y$		$\begin{vmatrix}0&\bar{1}&0\\1&\bar{1}&0\\0&0&1\end{vmatrix}$ & $\begin{vmatrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&1\end{vmatrix}$	$hk\alpha$ $\bar{h}+\bar{k},k,\alpha$ $h+k,\bar{h},\alpha$ $k,\bar{h}+\bar{k},\alpha$ $h,\bar{h}+\bar{k},\alpha$ $\bar{k}\bar{h}\alpha$ $\bar{h}+\bar{k},h,\alpha$ $\bar{h}\bar{k}\alpha$ $h+k,\bar{k},\alpha$ $kh\alpha$ $\bar{k},h+k,\alpha$ $\bar{h},h+k,\alpha$		$\boxed{6m}$

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