20.1-11 TOWARDS A BIOLOGICAL CRYSTALLOGRAPHY -THE CRYSTALLOGRAPHY OF QUASI-EQUIVALENCE. A.L.Mackay, Dept. of Crystallography, Birkbeck College, (Univ. of London), Malet Street, London WC1E 7HX.

It is characteristic of biological structures that strict equivalence, because of the small number of units, is replaced by quasi-equivalence. The configuration space has no dominating minimum and there are many quasi-equivalent minima. Accordingly, the pathways through the configuration landscape become important and the concept of information enters. Cellular automata are mathematical structures assembled by rules which are more general than the repetition rules of the space-groups. They can be extended to include biological morphogenesis (A.G.Jacobson and R.Gordon, Jour. Exp. Zoology, 197, 191-246 (1976). An example is given of a non-periodic pattern, which might be called a quasi-space-group (A.L.Mackay, Physics Bull. 495-7, (Nov.1976)). This is generated by a simple recursive rule and shows local symmetry of limited range. It is also hierarchic in structure, and may represent a first step out of the formalism of classical crystallography towards a modern version of D'Arcy Thompson's 'Growth and Form'. The pattern itself in 2 and 3 dimensions presents interesting mathematical problems, in its Fourier transform, and generally. There are connections between it and clusters on a variety of scales examined both theoretically and experimentally. (M.R.Hoare, Adv. Chem. Phys., 40, 49-135, (1979)).

Table I

Origin of next packing layer	Stacking symbol	TWO-DIMENSIONAL SPACE GROUPS AND SUBGROUPS														
		17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2
		p6m	p6	p31m	p3m1	p3	p4g	p4m	p4	cmm	pgg	pmg	pmm	cm	pg	pm	p2
0,0	s	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2
½,½	f	g	2	$\bar{5}$*	$\bar{5}$	1	12	11	10	9	8	7	6	5	4	3	2
0,½	b_y	g	2	5	5*	1	8	6	2	9	8	7	6	5	4	3	2
½,0	b_x	g	2	5*	5	1	8	6	2	9	8	7	6	5	4	3	2
⅓,⅔	c	14	13	13	14	13	$\bar{5}$	$\bar{5}$	1	1	1	1	1	1	1	1	1
0,q	m_y	5	1	5	(a)	1	4	3	1	5	4	3	3	5	4	3	1
p,0	m_x	5*	1	5*	(a)	1	4*	3*	1	5*	4*	4*	3*	1	1	1	1
p,q	m	(b)	1	(a)	(a)	1	(a)	(a)	1	(c)	1	1	1	(a)	1	1	1

(a)-one, (b)-two, (c)-three, particular cases with higher symmetry. One bar means that [11] of simple cell is taken as x-axis of double cell; underline, double cell; *, permutation of axes $x \rightleftarrows y$.

20.2-01 GROUP-SUBGROUP RELATIONS BETWEEN PLANE GROUPS AS INDUCED BY THE STACKING OF IDENTICAL PACKING LAYERS - by M.O. Figueiredo, J.I.C.U., Alameda D.Afonso Henriques, 41 - 4ºE, 1000 Lisboa, Portugal

Computer program VOID (in APL) calculates the positions and the radii of all interstices between two packing layers (Langlet, Figueiredo & Lima-de-Faria, J. Appl. Cryst. (1977) 10,21). Computing time should be considerably reduced if only the symmetrically independent voids were calculated, and then repeated by symmetry. It is therefore necessary to know in advance the symmetry group of the final pattern of interstices, which can be deduced from the plane group of the packing layer as a function of the stacking vector relating it to the forthcoming layer. A table of such group-subgroup relations between two-dimensional space groups is presented (table I), and the results compared with a previous complete list of subgroups (Sayari, Billiet & Zarrouk, Acta Cryst (1978) A34, 553). Applications are illustrated by various close-packing layers and corresponding condensed-model (Lima-de-Faria, Zeit. Krist. (1965) 122,346) sheets, whose automatic plotting is the final purpose of VOID program. Further use of present results is foreseen in the field of systematics of crystal structures for the improvement of layer-stacking symbolism, in connexion with special projections of three-dimensional space groups.

20.2-02 ORIGIN-SHIFT GROUPS? By S.C.Nyburg and W. Wong-Ng, Department of Chemistry, University of Toronto, Toronto, Canada M5S 1A1.

Space groups are a manifestation of a physical requirement, namely, that the Gibbs free energy of the crystal (in its most stable polymorphic phase) shall be a minimum. One might expect this could only be realized if every atomic/molecular motif was located in the same environment. However, a widely known exception is where the unit cell contains some molecules in equivalent positions and others in special positions. The environments of these two types of molecule cannot be the same. Another possibilty arises, at least in principle, in structures where the number of molecules per cell is some multiple of the number of equivalent positions. Each assembly of equivalently related molecules must be related by the equivalent positions of the space group, but these positions need not utilize the same (or an equivalent) origin. If this were to happen and, admittedly, free energy considerations may militate against it, it would be difficult to solve the structure. Although the Laue symmetry and systematic absences are not affected, the phase relations between related reflections are destroyed. (We can even contemplate the bizarre possibility of the various assemblies of equivalently related molecules belonging to different space groups so long as the Laue symmetry and systematic absences were the same). Destruction of phase relations could prevent the application of direct methods of structure solution.