Table 9.7.2.1. *Statistics of the use of Wyckoff positions of specified symmetry $\mathcal{G}$ in the homomolecular organic crystals, based on the data by Belsky, Zorkaya & Zorky (1995)*

$\mathcal{G}$	Space groups with positions of symmetry $\mathcal{G}$	Space groups actually occurring	Space groups using such positions
1	230	116	57
2	167	79	38
m	99	42	25
$\bar{1}$	38	28	10
3	57	18	7
4	24	6	4
$\bar{4}$	29	17	8
222	50	15	5
$mm2$	57	18	5
$2/m$	39	21	6
6	5	1	0
$\bar{6}$	8	3	1
32	22	5	1
$3m$	22	8	5
$\bar{3}$	14	7	4
422	9	1	1
$\bar{4}2m, \bar{4}m2$	19	5	3
$4mm$	8	3	0
$4/m$	7	2	1
mmm	16	3	2
23	12	3	2
622	2	1	0
$\bar{6}2m, \bar{6}m2$	5	1	1
$6mm$	2	0	0
$6/m$	2	1	0
$\bar{3}m$	8	3	1
$4/mmm$	4	2	1
432	5	0	0
$\bar{4}3m$	6	2	1
$m\bar{3}$	5	2	1
$6/mmm$	1	0	0
$m\bar{3}m$	3	2	2

9.7.2.1 indicates that there are 38 space groups with special positions of symmetry $\bar{1}$, that 28 of them have examples of structures of some kind, and that ten have structures in which the centre of symmetry is actually used by a molecule.

The three space groups with no special positions except those of symmetry $\bar{1}$ are very popular, whether or not the centre of symmetry is actually used by the molecule. The single criterion 'no special positions except possibly free centres of symmetry' thus selects the space groups favoured by structures in which inherent molecular symmetry is not used.

9.7.4.3. *Other symmetries*

Table 9.7.2.1 gives statistics for the number of space groups possessing Wyckoff positions of symmetry $\mathcal{G}$, where $\mathcal{G}$ is one of the 32 point groups, the number exhibiting structures of some kind, and the number in which the special position of symmetry $\mathcal{G}$ is actually used. It has to be remembered that this table represents the state of knowledge in 1994, that there may be small errors in the counts in the second column, and that new structures will gradually increase the numbers in the third and fourth columns. Nevertheless, some trends are clear. The arrangement of the point groups is in ascending order of their 'order' (Hahn, 1995, p. 781), and all numbers show a general decrease with increasing order. When molecular symmetry is used, the favourite is the diad axis 2, closely followed by the mirror plane m, with the centre of symmetry $\bar{1}$, the triad axis 3 and the tetrad inversion axis $\bar{4}$ trailing. It must also be remembered that these data are for numbers of *space groups*, not numbers of *structures*.

9.7.4.4. *Positions with the full symmetry of the geometric class*

The symmorphic space groups are in a one-to-one correspondence with the arithmetic crystal classes, and each has at least one Wyckoff position with the full symmetry of the geometric crystal class. It would thus be possible for each symmorphic space group to accommodate molecules with the full symmetry of the point group corresponding to the geometric crystal class. With the obvious exceptions of $P1$ and $P\bar{1}$, there seem to be no symmorphic space groups with primitive cells and one molecule only in the cell that do so, but the data of Belsky, Zorkaya &

references