time without a deterioration of the quality of the structure-factor set. The largest effect is obtained for crystals with a large unit cell, crystals having weak reflexions and those suffering from radiation damage.

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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1985). A**41**, 203-204

Revised space-group frequencies for organic compounds.*

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Abstract

In a recent paper Mighell, Himes & Rodgers [*Acta Cryst.* (1983), A**39**, 737-740] reported the space-group frequency for nearly 30 000 organic compounds in the *NBS Crystal Data Identification File* [(1982). JCPDS, Swarthmore, PA]. When the frequencies tabulated by Mighell *et al.* for those space groups that do not contain any operations of the second kind are revised somewhat different results are obtained. (Numbers given by Mighell *et al.* are given in parentheses.): 75% (75%) of compounds fall into only five space groups: $P2_1/c$, 29·2% (36.0%), $P2_12_12_1$, 18·8% (11·6%), $P\bar{1}$, 11·1% (13·7%), $P2_1$, 10·9% (6.7%) and $C2/c$, 5·4% (6·6%); 12(16) space groups account for 87% (90%) of the compounds.

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Making use of the *NBS Crystal Data Identification File* (1982), Mighell, Himes & Rodgers (1983) calculated the

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Table 1. *Revised frequencies for 53 space groups*

Not including 12 unoccupied space groups.

Space group	Number	Revised frequency	Space group	Number	Revised frequency
$P1$	1	610	$I4_322$	98	2
$P2$	3	22	$P3$	143	20
$P2_1$	4	3914	$P3_1$	144	31
$C2$	5	546	$P3_2$	145	31
$P222$	16	14	$R3$	146	80
$P222_1$	17	18	$P321$	150	10
$P2_12_12$	18	374	$P3_121$	152	35
$P2_12_12_1$	19	6718	$P3_221$	154	35
$C222_1$	20	172	$R32$	155	46
$C222$	21	10	$P6_1$	169	30
$I222$	23	14	$P6_5$	170	30
$I2_12_12_1$	24	10	$P6_2$	171	5
$P4$	75	2	$P6_4$	172	5
$P4_1$	76	54	$P6_3$	173	66
$P4_2$	77	6	$P622$	177	4
$P4_3$	78	54	$P6_122$	178	7
$I4$	79	24	$P6_522$	179	7
$I4_3$	80	18	$P6_222$	180	5
$P422$	89	2	$P6_422$	181	5
$P42_12$	90	8	$P6_322$	182	12
$P4_122$	91	4	$I23$	197	6
$P4_12_12$	92	145	$P2_13$	198	30
$P4_222$	93	4	$F432$	209	2
$P4_22_12$	94	14	$F4_132$	210	6
$P4_322$	95	4	$P4_332$	212	2
$P4_32_12$	96	145	$P4_132$	213	2
$I422$	97	4			

Table 2. *The 12 space groups with the highest frequencies*

Space group	Number of entries	Percent of total	Space group	Number of entries	Percent of total
$P2_1/c$	10450	29·2	$P1$	610	1·7
$P2_12_12_1$	6718	18·8	*Pnma*	548	1·5
$P\bar{1}$	3986	11·1	$C2$	546	1·5
$P2_1$	3914	10·9	$Pna2_1$	513	1·4
$C2/c$	1930	5·4	$P2_12_12$	374	1·0
Pbca	1261	3·5	*Pbcn*	341	1·0

frequency of occurrence for each of the 230 space groups. This file is based on structures that have been reported in the literature.

However, for some compounds a space-group determination has an added bonus in that a second space-group determination is automatically made. Thus, when Shoemaker, Schomaker, Donohue & Corey (1950) established the space group of L-threonine as $P2_12_12_1$ they automatically established the space group of D-threonine also as $P2_12_12_1$, without ever seeing any of that substance. On the reasonable assumption that, because we are concerned here with organic molecules, all of the 3359 crystals in the file that were found to have space group $P2_12_12_1$ will have a corresponding enantiomer with that space group, so the frequency should be doubled. This same situation will obtain for the other 64 space groups that contain no symmetry operations of the second kind. These are those space groups belonging to point groups 1, 2, 222, 4, 422, 3, 32, 6, 622, 23 and 432. In the case of the ten enantiomeric pairs, for example, $P4_1$ and $P4_3$, for which 47 crystals were found for the former, and seven for the latter, the results should be combined, to give 54 for each for that pair; similar calculations were made for the other nine pairs. For the remaining space groups the number of entries should be doubled. The revised frequencies are presented in Table 1. This table should be combined with the unrevised values of Table 1 of Mighell *et al.* to give the complete set of frequencies for the 230 space groups. The total number of crystals is increased from 29 059 to 35 771.

In the unlikely event that two different sets of investigators reported determinations, say, of D-tartaric acid in one laboratory and L-tartaric acid from a second laboratory, the space group for both will already be in the file, and the frequency number for $P2_1$ will be over-revised. I believe that the chance that this has happened is very small indeed.

The rank order of the first five most populous space groups is changed, with $P2_12_12_1$ now in second place instead of $P\bar{1}$. The first 12 in the list are presented in Table 2. Each of the remaining 218 space groups has less than 1% of the total.

The precautionary remarks of Mighell *et al.* still, of course, apply.

I thank Dr Richard E. Marsh for interesting suggestions.

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A comment on the calculation of rocking curves near the critical voltage in electron diffraction.

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Abstract

Several authors have reported the occurrence of a sharp peak doublet in certain rocking curves calculated for voltages near the critical voltage in electron diffraction. It is shown that such peaks are only artefacts due to the use of an approximation that becomes invalid under illumination conditions for which the main Bloch waves are nearly degenerate.

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