of the complement structure from a given excess points Patterson transform, is best done in terms of real electron density. In terms of real electron density, if $\mathbf{F}_s$ is the structure factor for the sub-cells and $\mathbf{F}_c$ for the complement structure, then at the sub-cell reciprocal lattice points

$$I_{s+c} = (\mathbf{F}_s + \mathbf{F}_c)^2 = F_s^2 + 2\mathbf{F}_s . \mathbf{F}_c + F_c^2 .$$

The F_c^2, together with those for the excess points, are the transform of the Patterson function of the (real) complement structure. $F_s^2 + 2\mathbf{F}_s . \mathbf{F}_c$ transforms to the Patterson function of the sub-structure plus the cross vectors between the sub-structure and the complement structure. The transform of the excess points, weighted with the intensities, is thus the scaled down version of the Patterson function of the complement structure, with a background of overlapping negative Patterson functions of the complement structure, exactly analogous to the Fourier case. However, even in the most favourable case of a Patterson function, it will be necessary to allow for the large negative origin peaks at the sub-cell lattice points, and where the superstructure is due to small displacements from ideal positions the cluster of positive and negative peaks round the ideal position will tend to cancel out. This is a particular case of the general possibility, which occurs in the case of Patterson functions, of coincident or near coincident positive and negative peaks. Projections will tend to suffer more from such cancellations than three-dimensional syntheses.

The referee's help, especially in pointing out many of the implications of the negative electron density approach, is gratefully acknowledged.

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Single-crystal studies of β-F_2 and of γ-O_2.

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Techniques for the growth, orientation and X-ray diffraction study of single crystals of β-N_2 (Streib & Lipscomb, 1962; Streib, Jordan & Lipscomb, 1962) have been extended to single crystal studies of β-F_2 at 50 °K and γ-O_2 at 50 °K. These phases have, surprisingly, the same structure-type (Fig. 1). Unit-cell dimensions are $a = 6{\cdot}67 \pm 0{\cdot}07$ Å for β-F_2 and $6{\cdot}83 \pm 0{\cdot}05$ Å for γ-O_2, and there are eight diatomic molecules in the unit cell. Systematic absences of hhl when l is odd suggest space groups $P\bar{4}3n$ or $Pm3n$, but our results indicate an orientationally disordered structure in $Pm3n$.

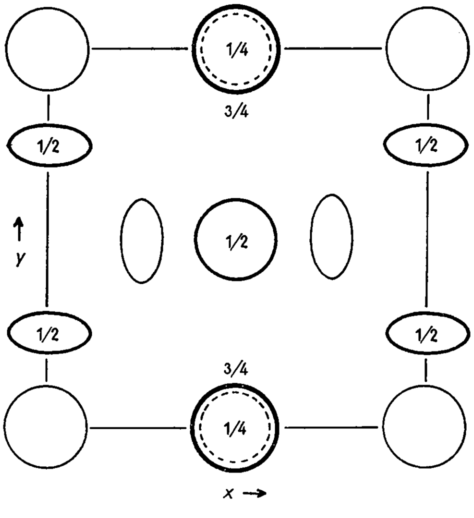

Fig. 1. Crystal structure of β-F_2 and of γ-O_2. Out-of-plane coordinates are indicated for each molecular center, except for those at $z = 0$, which are unlabeled. The two molecules at 000 and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ are approximately spherically disordered. The other six molecules, at $\frac{1}{4}\frac{1}{2}0$, $0\frac{1}{4}\frac{1}{2}$, $\frac{1}{2}0\frac{1}{4}$, $\frac{3}{4}\frac{1}{2}0$, $0\frac{3}{4}\frac{1}{2}$ and $\frac{1}{2}0\frac{3}{4}$, show an oblate spheroidal distribution of electron density such that the ratio of major to minor axis is about two. Minor axes are aligned along the shortest intermolecular contacts (3·3 Å in F_2, 3·4 Å in O_2) along $x(y = \frac{1}{2}, z = 0)$, along $y(x = 0, z = \frac{1}{2})$ and along $z(x = \frac{1}{2}, y = 0)$. Bond distances of 1·21 Å for O_2 and 1·42 Å for F_2 were assumed.

In β-F_2 each F_2 at 000 or at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ has 12 F_2 neighbors at 3·7 Å between molecular centers. Each of the other F_2's has $2F_2$'s at 3·3 Å, 4 F_2's at 3·7 Å and 8 F_2's at 4·1 Å. Van der Waals contacts are 2·7 Å if two F_2's have their molecular axes perpendicular to, or 4·1 Å if their axes are along, the line of contact. Thus, the disorder is strongly hindered along the infinite linear chains of F_2 molecules separated by 3·3 Å. We have verified the presence of a major transition, suspected by Murphy & Rubin (1952) because of an entropy discrepancy, and found by Hu, White & Johnston (1953), but we have obtained only powder photographs of α-F_2 by cooling single crystals of β-F_2 through the transition point at 45·55 °K.

The essential identity of the γ-O_2 and β-F_2 structures makes untenable any description of γ-O_2 based upon dimers of O_2 (Ruhemann, 1932; Vegard, 1935), and further suggests that the unusual magnetic properties of γ-O_2 (Kanda, Haseda & Otsubo, 1955) do not determine the structure. The presence of infinite linear chains of O_2 molecules is consistent with the very short range interactions suspected by Kanda *et al.* (1955) (Knobler, 1961; Lien & Phillips, 1961), but this structure raises serious questions about the existence of dimers in the other solid phases and in solution (Lewis, 1924; Pauling, 1960). Even the nearly spherically disordered molecules at 000 and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ cannot have more than about one-tenth of the contribution of free O_2 molecules (Van Vleck, 1932) to the magnetic susceptibility of β-O_2. Magnetic and crystallographic studies of dilute solutions of O_2 in β-F_2 or in β-N_2 would be of interest in elucidating the disorder and interactions.

Table 1. *Structure factors for* β-F_2 and γ-O_2

	β–F_2		γ–O_2	
hkl	F_o	F_c	F_o	F_c
110	—	1·8	—	1·8
200	20·3	17·4	34·7	34·8
210	23·2	22·9	37·1	40·9
211	22·2	21·2	36·8	38·4
220	5·4	−5·7	9·9	−7·5
310	2·0	2·2	4·9	3·3
222	6·0	−2·6	17·9	−13·5
320	3·4	−1·6	13·9	−9·9
321	3·7	3·5	13·7	12·4
400	7·4	7·2	20·9	22·7
410	6·0	−5·5	12·2	−10·3
411	3·1	−4·1	7·3	−7·2
330	3·6	3·2	8·4	5·3
420	2·2	1·2	10·6	7·4
421	2·3	1·9	9·4	8·0
332	1·7	1·1	4·4	1·7
422	3·5	3·1	7·9	7·2
430	2·5	−3·0	6·3	−7·0
510	—	−0·8	—	0·1
431	1·7	−0·5	4·2	−1·8
520	1·9	0·8	4·2	1·6
432	2·0	1·7	—	1·3
521	1·3	−0·8	—	−0·5
440	2·5	−1·5	—	−0·9
530	1·3	0·9	—	2·9
433	—	0·7	—	1·2
531	—	0·0	—	0·0
600	2·1	−2·1	7·8	−7·3
442	2·1	0·3	1·7	2·8
610	—	1·3	—	4·4
611	—	0·1	4·4	2·5
532	1·7	−1·0	—	−2·7
620	1·9	−1·8	4·1	−6·0
621	—	0·4	4·3	−3·2
540	—	1·0	—	3·6
541	—	0·1	—	0·1
622	—	−0·2	—	−0·6
630	—	−0·2	—	−0·4
542	—	−1·0	—	−4·0
631	—	−0·1	—	0·6
444	2·6	−1·7	4·1	−6·3
632	—	0·3	2·9	2·4

The agreement obtained so far is about equally good for (*a*) spherically disordered O_2 (or F_2) at 000 and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ and cylindrically disordered O_2 in the other sites so that the bond lies in the plane of disorder ($R = 0{\cdot}16$), and (*b*) a statistical model in which the F atoms of the molecular twofold site are in 16-fold positions ($\frac{1}{4}$ F's on threefold axes), and the F atoms of the other molecules are in 24-fold positions ($\frac{1}{2}$ F's in the plane of disorder). Large isotropic temperature factors are also required for model (*b*), which also yields $R = 0{\cdot}16$ for either γ-O_2 or β-F_2 (Table 1). Three-dimensional electron density maps also indicate spherical disorder for the O_2's (F_2's) at 000 and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, but oblate spheroidal distributions for the other O_2's. Further studies of the many related types of disorder are in progress.

Note added in proof.— Later refinements have reduced *R* to 0·10 for β-F_2 and 0·13 for γ-O_2.

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On the symmetry of phases in the reciprocal lattice: a simple method.

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No mention is made in recent papers on reciprocal lattice symmetry (Bienenstock & Ewald, 1962; Jeffery, 1963) of the technique of structure factor algebra to find phase relations between structure factors. Our simple 'do-it-yourself method' uses the information already contained in *International Tables for X-ray Crystallography* (1952). We only require the knowledge of the so called general positions which is equivalent to the knowledge of the symmetry elements. Indeed *to every symmetry operation* $\mathbf{r} \rightarrow \mathbf{r}'$ *corresponds a phase relation in reciprocal space.*

Let us illustrate the structure factor algebra method by the example of space group $P4_322\,(D_4^7)$ No. 95 where