For a one-dimensional space of transformation only two sets of symmetry groups exist, with two groups each:

the space groups $p1$ and pm for $\mathscr{G}^1$ (G_1), and
the point groups (1) and (m) for $\mathscr{G}_1$ (G_{10}) .

The symbols for symmetry groups proposed here seem to us to have the following advantages: They are sufficiently similar to the international space group symbols to be easily understood and visualized, and the tables of equivalent positions *etc.* given in *International Tables* can be used almost as they stand for the corresponding symmetry groups of all sets.

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A Scattering Curve for a Rotating Methane Molecule

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Various scattering factor curves have been calculated for a rotating methane molecule in an attempt to elucidate the effect of slightly different interatomic distances and angular terms. It is concluded that the effect of using slightly different interatomic distances is obscured by effects caused by different methods of obtaining the wave functions, while in the case of methane and, presumably, ammonium the effect of the angular terms is small.

Davis & Whitaker (1966) reported figures for a scattering curve for a spherically symmetrical ammonium group. The scattering curves were calculated for the Hartree self-consistent wave functions of Bernal & Massey (1954) and the analytical wave functions with exchange of Bernal (1953). The values of the scattering factors from these wave functions differed by up to 10% although both wave functions were calculated for the same nitrogen–hydrogen distance of 0·972 Å. This value is somewhat lower than the average value obtained in practice: 1·033 Å (*International Tables for X-ray Crystallography*, 1962, p. 270).

In an attempt to estimate the effect of small differences of interatomic distances on the scattering curves, these have been calculated for a rotating methane molecule.

There are two wave functions for methane comparable with those for ammonium, namely; the Hartree self-consistent wave functions of Buckingham, Massey & Tibbs (1941), calculated assuming a carbon–hydrogen distance of 1·056 Å and the analytical wave functions including exchange of Bernal (1953), calculated assuming a carbon–hydrogen distance of 1·043 Å.

The scattering curve based on the wave functions of Buckingham, Massey & Tibbs (1941) has already been reported (Banyard & March, 1956). However, it has been recalculated for ease in comparison with the other scattering curves; the ammonium wave functions of Bernal & Massey (1954) were calculated by the same method. Bernal (1953) used the same technique for the wave functions of both ammonium and methane. Thus it was thought that comparison of the various curves for ammonium and methane may give an indication as to the effect of slight differences of interatomic distances on the scattering curves. Incidentally, the interatomic distances for methane for which the wave functions were calculated are all considerably less than the average experimental value 1·091 Å (*International Tables for X-ray Crystallography*, 1962, p. 276).

In addition to these wave functions the Hartree–Fock self-consistent wave functions have also been calculated (Mills, 1958) assuming an interatomic distance of 1·056 Å and, in addition, Mills (1961) estimated the effect of the tetrahedral symmetry of the molecule on the radial density distribution (angular terms). The scattering curves for both these models have been calculated to estimate the effect of including the angular terms.

The electron density distributions of these wave-functions are given in Fig. 1; as expected, the effect of using a smaller interatomic distance causes the electron cloud to be contracted; exchange has a similar although smaller effect, while the effect of the angular terms is to make the electron cloud slightly more diffuse. The last conclusion was also obtained by Banyard & March (1961), but it appears that their conclusions were based on the incorrect angular terms given by Mills (1958). These have now been corrected (Mills, 1961).

However, in the case of ammonium, the use of analytical wave functions gives a contracted electron cloud compared with Hartree wave functions even when the same interatomic distance is used in both (Banyard & March, 1961).

To estimate the effect of these different distances on the scattering curves the latter were obtained by use of the formula

$$f=\int_0^\infty 4\pi r^2\varrho(r)\,\frac{\sin\mu r}{\mu r}\,dr$$

(James, 1948) where $\mu=4\pi\sin\theta/\lambda$ and $\varrho(r)$ is the electron density at a distance r. The integral was evaluated by repeated use of the Newton–Coates seven point formula at intervals of $0{\cdot}02a_0$.

The figures for the scattering factors for methane are given in Table 1 together with those for carbon (Freeman, 1959; *International Tables for X-ray Crystallography*, 1962, p. 202). The values of the scattering factors for $\sin\theta/\lambda=0$ are 10·003, 10·000, 9·999 and 10·000 for wave functions of Buckingham, Massey & Tibbs (1941), Bernal (1953), Mills (1958) excluding angular terms and Mills (1958, 1961) including angular terms respectively. Thus it would appear that the errors in the scattering factors are in the third decimal place, assuming that the wave functions are correct. However, this error is so small that it does not affect the remaining discussion.

Comparison of the scattering factor curves for methane, obtained from the wave functions of Buckingham, Massey & Tibbs (1941) and Bernal (1953) with each other, gives differences comparable to the differences obtained when the ammonium scattering factor curves are compared (Davis & Whitaker, 1966). There are some differences between the comparisons which may be due to the use of a different carbon–hydrogen interatomic distance, but these are small compared with the differences obtained by using different wave functions. Hence it appears that more reliable wave functions are required before the effect of incorrect interatomic distances can be assessed.

If the scattering factor curves from the Hartree–Fock self-consistent wave functions excluding (Mills, 1958) and including (Mills, 1958, 1961) the angular terms are compared, it is found that the differences are small, less than 1%. However, the methane molecule has high symmetry and for less symmetrical groups the effect of the angular terms will be larger. Presumably, in the case of the ammonium ion, which has the same symmetry as the methane molecule, the effect of the angular terms would also be small.

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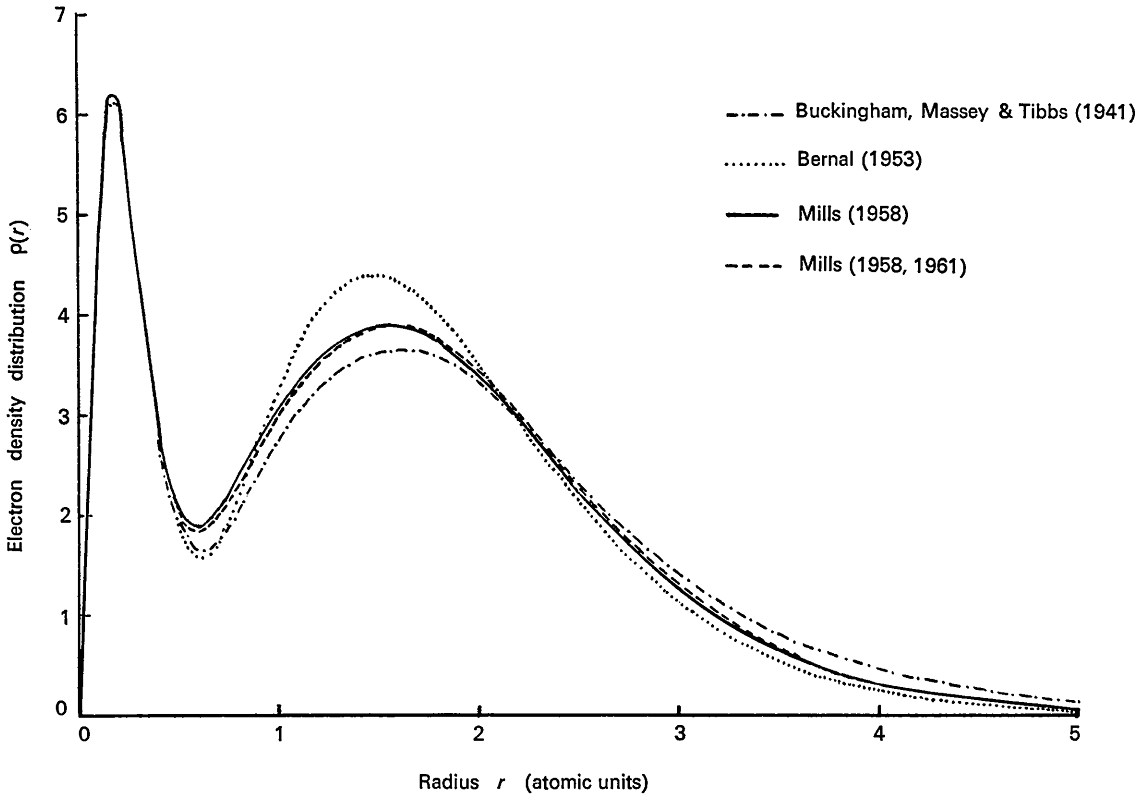

Fig. 1. Radial distribution curves for methane.

Table 1. *Scattering factors for methane and carbon*

$\frac{\sin\theta}{\lambda}$	Methane Buckingham Massey & Tibbs (1941)	Methane Bernal (1953)	Methane Mills (1958)	Methane Mills (1961)	Carbon International Tables (1962)
0·00	10·003	10·000	9·999	10·000	6·000
0·05	9·273	9·414	9·371	9·369	5·760
0·10	7·527	7·920	7·801	7·789	5·126
0·15	5·613	6·099	5·954	5·932	4·358
0·20	4·069	4·461	4·366	4·339	3·581
0·25	3·020	3·243	3·232	3·205	2·979
0·30	2·382	2·449	2·514	2·493	2·502
0·35	2·022	1·983	2·098	2·084	2·165
0·40	1·826	1·728	1·868	1·861	1·950
0·45	1·715	1·596	1·738	1·737	—
0·50	1·644	1·527	1·655	1·657	1·685
0·55	1·587	1·486	1·591	1·594	—
0·60	1·534	1·454	1·534	1·536	1·536
0·65	1·480	1·422	1·478	1·479	—
0·70	1·425	1·386	1·422	1·423	1·426
0·75	1·371	1·345	1·366	1·366	—
0·80	1·317	1·299	1·311	1·310	1·322
0·85	1·263	1·250	1·257	1·257	—
0·90	1·210	1·199	1·204	1·203	1·218
0·95	1·157	1·146	1·151	1·151	—
1·00	1·104	1·092	1·098	1·098	1·114
1·05	1·052	1·039	1·046	1·046	—
1·10	1·000	0·986	0·996	0·996	1·012
1·15	0·950	0·934	0·946	0·946	—
1·20	0·901	0·884	0·898	0·898	—
1·25	0·854	0·836	0·852	0·851	—
1·30	0·808	0·790	0·807	0·806	0·821
1·35	0·765	0·746	0·764	0·763	—
1·40	0·723	0·703	0·723	0·722	—
1·45	0·683	0·663	0·683	0·683	—
1·50	0·646	0·625	0·646	0·646	0·659
1·55	0·610	0·589	0·611	0·611	—
1·60	0·576	0·555	0·577	0·577	—
1·65	0·544	0·522	0·545	0·545	—
1·70	0·514	0·492	0·515	0·514	0·524
1·75	0·485	0·463	0·486	0·486	—
1·80	0·458	0·436	0·459	0·459	—
1·85	0·433	0·411	0·434	0·434	—
1·90	0·409	0·387	0·410	0·410	0·419

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Magnetic Symmetry of Vivianite $Fe_3(PO_4)_2.8H_2O$

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Possible magnetic space groups for antiferromagnetic vivianite, $Fe_3(PO_4)_2.8H_2O$, are derived on the basis of nuclear magnetic resonance measurements. The allowed space groups are P_A2_1/c and C_c2/c. The spin configurations corresponding to these space groups are discussed.

In 1961, possible magnetic space groups for antiferromagnetic vivianite, $Fe_3(PO_4)_2.8H_2O$, were derived by the author on the basis of nuclear magnetic resonance data of the protons and phosphorus nuclei (van der Lugt & Poulis, 1961). The actual derivation was published in Dutch (van der Lugt, 1961) and is not readily