Table 3 (*cont.*)

Number of lines (1)	Intensity* (2)	Spacing observed (3)	$Q(1/d_{hkl}^2)$ Observed (4)	Calculated (5)	Indices (6)
36	*vw*	1·628 Å	0·3773	0·3775	0,11,0
				0·3779	234
37	*vw*	1·602	0·3897	0·3891	144
				0·3896	563; 4,10,1
				0·3904	733
38	*vw*(broad)	1·527	0·4289	0·4283	11,0,0
				0·4286	663
39	*vw*	1·443	0·4802	0·4799	364
40	*vw*	1·382	0·5236	0·5234	6,10,2
				0·5235	972

* *vs*, very strong; *s*, strong; *m*, medium; *w*, weak; *vw*, very weak.

be 0·00354, 0·00312 and 0·02098 respectively. There is good agreement between the observed and calculated Q values as shown in Table 3. The unit-cell dimensions are: $a=16{\cdot}81$, $b=17{\cdot}90$, $c=6{\cdot}90_4$ Å. The density was measured with a specific-gravity bottle of very low weight, designed specially for the purpose, and is found to be 1·27 g.cm^{-3}. The density, calculated for eight molecules per unit-cell is 1·30 g.cm^{-3}. As can be seen from Table 3, systematic absences of the reflexions could not be assigned owing to the limited number of unresolved reflexions. The space group *Pmmm* is thus tentatively assigned to the crystal.

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The crystal structure of Mg_3NF_3.

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Mg_3NF_3 is cubic with $a=4{\cdot}216$ Å, space group *Pm*3*m*. The structure is related to the NaCl-structure type. The anion arrangement is ordered.

Two new nitride fluorides of magnesium are formed when nitrogen is passed over mixtures of Mg and MgF_2 at temperatures of 900–1050°C. One of them, Mg_3NF_3, is cubic with $a=4{\cdot}216$ Å, $D_m=3{\cdot}16$, $D_c=3{\cdot}19$ g.cm^{-3} and $Z=1$. The space group is *Pm*3*m*, with three Mg atoms in the 3(*c*) positions, three F atoms in 3(*d*) and one N atom in 1(*b*).

The R value for 18 reflexions, collected with an X-ray powder diffractometer with Cu $K\alpha$ radiation, was 0·022. The atomic form factors used were those for Mg^{2+}, F^- and N^{3-} obtained from *International Tables for X-ray Crystallography* (1962); the N^{3-} form factors were constructed from the N and N^- curves given therein. If the anions were assumed to be randomly distributed over the 3(*d*) and 1(*b*) positions, the R value increased to 0·053.

A magnesium atom is octahedrally surrounded by four fluorine and two nitrogen atoms at equal distances of 2·108 Å. The nitrogen atom is octahedrally surrounded by six cations, as in Ca_2N (Keve & Skapski, 1968). A fluorine atom is surrounded by four cations in a square-planar arrangement. The structure of Mg_3NF_3 is similar to the MgO or NaCl structure type, but with one of the cation positions (000) empty in an ordered way. The anion arrangement is intact, although the two different anions are ordered.

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