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A barium-iron-oxide with the perovskite structure.

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A perovskite-like structure having the composition $Ba_8Fe_8O_{21}$ has been reported as a result of an investigation of barium–iron–oxygen compounds (Erchak, Fankuchen & Ward, 1946). Later the Ba–Co–O system was examined and three new phases were found; $BaCoO_{2\cdot72}$, $BaCoO_{2\cdot31}$, and $BaCoO_{2\cdot23}$. The latter has the perovskite structure (Strauss, Fankuchen & Ward, 1951). Rare earth ferrites ($A^{3+}B^{3+}O_3^{6-}$) in which iron has a valence of 3^+ have been demonstrated (Geller & Wood, 1956). Barium manganite (Jonker & van Santen, 1950) and strontium cobaltite (Jonker & van Santen, 1953) have the perovskite structure with the transition metal in a valence state of $4^+(A^{2+}B^{4+}O_3^{6-})$.

In view of the above it was of interest to know if a reaction could be found that would produce a stoichiometric $BaFeO_3$ with the perovskite structure. Reacting various oxides, hydroxides and carbonates of barium and iron has to date failed to produce a compound with the perovskite structure. We have succeeded in obtaining a barium–iron–oxide with the perovskite structure by modifying the method of Clabaugh, Swiggard & Gilchrist (1956). This method was originally developed to produce a high purity barium titanate and consists in precipitating barium titanyl oxalate tetrahydrate followed by calcination.

The powder data listed in Table 1 were obtained with a Philips wide angle goniometer and Cu $K\alpha$ radiation. The data for cubic barium titanate are included in Table 1 as a basis for comparison. From this data it would follow that the new compound is isostructural with cubic $BaTiO_3$ and is stoichiometric $BaFeO_3$ with iron in a valence state of 4^+.

The deviation from the procedure of Clabaugh, Swiggard & Gilchrist consists in starting with a ratio of barium to iron of 1·5 to 1 instead of the ratio near 1 to 1 used with barium and titanium. The oxalate was precipitated at 50 °C. and calcined at 700 °C.

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Table 1. *Powder data*

	$BaFeO_3$				$BaTiO_3$		
			Intensities			Intensities	
hkl	*d*	a_0	Observed	Calculated	*d*	Observed	Calculated
100	4·012 Å	4·012 Å	8	14	4·017 Å	19	20
110	2·837	4·012	100	100	2·841	100	100
111	2·325	4·027	18	20	2·319	29	25
200	2·006	4·012	31	33	2·009	36	33
210	1·788	3·998	7	7	1·797	11	10
211	1·637	4·010	31	37	1·640	41	37
220	1·414	3·999	15	19	1·420	20	20
300, 221	1·338	4·014	4	3	1·339	6	4
310	1·272	4·022	11	16	1·270	16	16
311	1·211	4·016	7	6	1·211	8	8
222	1·159	4·015	4	6	1·160	7	7

Note: A Wilson Powder Camera was used to determine the *d* (Å) values.

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Histamine. — Preliminary X-ray studies of the crystalline free base.

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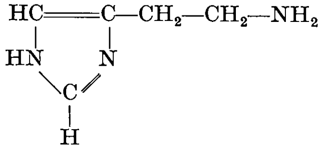

This is a report on the preparation and crystal structure of histamine free base ($C_5N_3H_9$) and is preliminary to the complete molecular structure determination of the free base. Neither the crystal structure nor the interplanar spacings of anhydrous histamine free base have been previously reported. However, the structure of the