TABLE 2

Phase A						Phase B		Phase C	
d, Å	hkl	I/I_1	d, Å	hkl	I/I_1	d, Å	I/I_1	d, Å	I/I_1
6.48	011	4	1.790	142	16	6.45	70	4.31	20
5.86	002	7	1.744	332	17	5.79	5	4.21	30
3.99	112	23	1.737	240.332	12	5.28	5	4.17	25
3.87	200	3	1.697	143.135	12	4.57	40	3.97	50
			1.615	044	1	3.87	20	3.358	100
3.675	021	2	1.580	243,144	10	3.77	40	3.302	25
3.461	013,120	20	1.550	334	2	3.71	40	3.227	50
3.314	121	20	1.537	340	2	3.62	20	3.175	50
3.223	022	20	1.525	150	2	3.51	30	2.978	30
			1.503	342	2	3.44	80	2.894	5
2.986	122	100	1.490	244	8	3.336	90	2.747	20
2.916	004	23	1.472	153	2	3.234	100	2.592	25
2.738	014	3	1.460	008	3	3.038	70	2.508	10
2.592	114	17	1.440	343.335	10	3.000	100	2.453	20
2.524	031	5	1.398	252	10	2.903	60	2.436	30
2.455	130	35	1.371	344.440	5	2.763	50	2.392	25
2.328	024	1	1.353	253.154	5	2.578	90	2.332	25
2.257	132	9	1.331	336.442	10	2.327	15	2.281	10
2.237	015	42	1.290		15	2.217	15	2.243	25
2.161	230.033	5				2.166	40	2.222	20
2.116	231	1				2.010	5	2.193	10
1.996	224	3				1.958	5	2.085	20
1.938	040	9				1.872	5	2.032	30
1.877	140.233	25						1.834	26
1.841	042	14						1.787	20

[9], condensation of SiO_4 tetrahedra led to formation of an $[Si_4O_{10}]_\infty$ network. It has been hypothesized that the structure of $Ba_2Si_3O_8$ contains complex chains [10], while an (Si_3O_9) ring is expected in the α-$BaSiO_3$ structure by analogy with $SrGeO_3$ [11].

The phase transition under investigation was determined from the change in the BaO/H_2O ratio, but there is no doubt that phase formation in the $BaO-SiO_2-H_2O$ system at BaO/H_2O = const also depends on the BaO/SiO_2 ratio. Thus, when the silica content of the charge was reduced, both carbonite ($BaSi_2O_5$) and $Ba_2Si_3O_8$ crystallized (experiments 1-3). An excess of barium oxide led to formation of α-$BaSiO_3$ (experiments 4 and 7), while a further increase in the amount of BaO caused crystallization of a previously unknown barium silicate, the A phase (experiment 17). Detailed morphological and x-ray diffraction analyses (Table 2) made it possible to detect two additional "new" phases among the crystalline synthetic products: phase B (experiment 5) and phase C (experiments 6, 8, 9, 13, and 14). Single crystals of $Ba_2TiSi_2O_8$ were found in the titanium-lined autoclaves [12].

Experimental x-ray data for these phases were obtained from their Laue powder patterns, oscillatory diffraction patterns, and layer-line scanning patterns (using a KFOR chamber with Mo radiation). The unit-cell parameters were determined more precisely in a DRON-1 diffractometer (MoCu radia-

tion). The x-ray diffraction analysis was made in a URS-50IM apparatus (CuKα radiation). The faceted single crystals were measured in a GD-1 optical goniometer. The crystal arrangement was the same as for the x-ray analysis. The density of phase A was determined by hydrostatic weighing and its optical constants by focal screening. Table 2 gives the interplanar distances for the new phases, which are briefly described below.

Phase A: $5BaO \cdot 4SiO_2 \cdot 1.2H_2O$.[1] Short, transparent, colorless prismatic crystals. Tetragonal habit. Lattice constants: $a = 7.745 \pm 0.006$ Å, c = 11.680 ± 0.006 Å, Z = 2. Possible Fedorov groups: P4/mnc, P4nc; $\rho_e = 4.64 \pm 0.02$ g/cm^3, $\rho_{x\ ray} = 4.84 \pm 0.03$ g/cm^3. Crystals uniaxial, positive; refractive indices $n_e = 1.744 \pm 0.002$ and $n_o = 1.730 \pm 0.002$. Basic forms: well-developed $\{100\}$ and $\{110\}$ tetragonal prisms and $\{203\}$ and $\{111\}$ tetragonal bipyramids; $\{120\}$ ditrigonal prism and pinacoid less characteristic (Fig. 1a). Phase A is also characterized by a certain number of twins.

Phase B. Composition unknown; individual crystals in prismatic system (Fig. 1b), rhombic habit. Lattice constants: $a = 13.048 \pm 0.005$ Å, b = 15.644 ± 0.006, c = 7.203 ± 0.003 Å. Fedorov group A2$_1$22. Refractive indices: $n_p = 1.585 \pm 0.003$, $n_g = 1.597 \pm 0.003$.

[1]The chemical analysis was performed by V. S. Bykova.