

pected anomaly was found: the very broad and strong absorption lies in the region of 400–1600 cm⁻¹ with its maximum at 900 cm⁻¹.

Judging from the results so far available, which are consistent with other Type A acid salts, it seems probable that the O(1)···O(1ⁱ) bond is not only crystallographically, but also truly, of the symmetrical single-minimum type. The problem of the symmetrical OHO bond is interesting, since a model of order-disorder type is accepted in most hydrogen-bonded ferroelectrics. Structure analysis in the ferroelectric phase (at about 80°K) is now in progress. A more detailed discussion will be given on the basis of the structures of the para- and ferroelectric phases.

I am very grateful to all the staff in this laboratory for their valuable discussion and cooperation. I also wish to thank Professor K. Nakatsu of Kwansei Gakuin University for his valuable discussion and suggestion on the symmetrical hydrogen bond, and Professor Y. Matsunaga and Professor E. Osawa for their courtesy in the measurement of the infrared spectra. Thanks are also due to Dr T. Sakurai for kindly giving the information on 'UNICS', and to the Computing Centre of the University of Tokyo and the Hokkaido University Computing Center for making the HITAC 5020E and the FACOM 230-60 computer available to me.

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Barium Aluminate Hydrates. V.* The Crystal Structure of γ -Ba[AlO(OH)₂]₂

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γ -BaO·Al₂O₃·2H₂O is orthorhombic, *Fdd2*, with $a=20.70$, $b=8.977$, $c=6.416$ Å, $Z=8$. X-ray structural analysis shows that it contains chains of composition [AlO(OH)₂]_∞, made up of tetrahedra sharing corners. Its formula should therefore be written γ -Ba[AlO(OH)₂]₂.

Introduction

Carlson & Wells (1948) were the first to produce monobarium aluminate dihydrate and their compound was

designated 'α' by Thilo & Gessner (1965) when a second polymorph ('β') was found. Ahmed & Dent Glasser (1970) solved the structure of the α-polymorph and (1971) prepared a third compound of the same empirical formula which they called 'γ'. This present work deals with the γ modification. Crystal data from Ahmed & Dent Glasser (1971) are reproduced in Table 1. The compound crystallizes as plates lying on (100).

* Part IV: Dent Glasser & Giovanoli, *Acta Cryst.* (1972). **B28**, 519.

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Table 1. Crystal data of $\gamma\text{-BaO}\cdot\text{Al}_2\text{O}_3\cdot 2\text{H}_2\text{O}$

a	$= 20.70 \pm 0.02 \text{ \AA}$
b	$= 8.977 \pm 0.004$
c	$= 6.416 \pm 0.003$
D_{obs}	$= 3.25 \text{ g.cm}^{-3}$
D_x	$= 3.35 \text{ g.cm}^{-3}$

Space group $Fdd2$ Unit cell content $\text{Ba}_8\text{Al}_{16}\text{O}_{48}\text{H}_{32}$

Experimental

Intensity data were collected using a Hilger and Watts Y190 automatic linear diffractometer with Mo $K\alpha$ radiation ($\lambda = 0.7107 \text{ \AA}$). The rotation axis of the crystal was c , and reflexions throughout one half of reciprocal space up to $l=8$ were measured. This gave a total of 1629 reflexions not systematically absent; agreement between equivalent reflexions was very good. After averaging equivalent reflexions a total of 529 reflexions remained, of which 71 were not considered to be significantly above background and were treated as 'unobserved'. Intensities were converted to structure factors in the usual way. No corrections were made for absorption or extinction. Data were processed on an ICL 4/50 computer, mainly using programs supplied by Dr F. R. Ahmed and collaborators of the National Research Council of Canada, and adapted for use on this machine by Mr J. S. Knowles of the Department of Computing, University of Aberdeen. Scattering factors for Ba^{2+} and Al^{3+} were taken from *International Tables for X-ray Crystallography* (1962). A curve for O^{2-} was constructed as described by Ahmed & Glasser (1970).

Structure determination

Approximate positions for the barium, aluminum and oxygen atoms were derived from the Patterson function and refined by the method of least squares (block-diagonal approximation). Reflexions were weighted according to $W = 1/\{1 + [(|F_o| - P_2)/P_1]^2\}$. P_1 and P_2 were chosen initially to give maximum weight to reflexions of moderate intensity; subsequently an error analysis showed that the scheme selected was reasonable.

The Patterson function could be satisfied by two solutions. One set of parameters refined readily to a

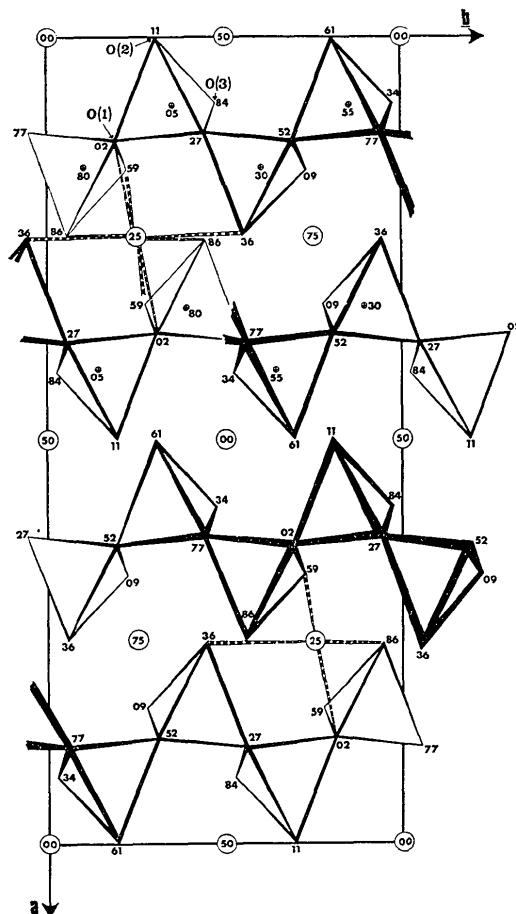


Fig. 1. The structure of $\gamma\text{-Ba}[\text{AlO(OH)}_2]_2$ projected down c ; heights are in $c/100$. Oxygen atoms are at the corners of the tetrahedra, and the heights of the corresponding aluminium atoms (small circles containing crosses) are shown in the upper half of the diagram. Large open circles indicate barium atoms. The upper half of the cell is drawn to emphasize the twofold axes on which the barium atoms lie; the lower emphasizes the perspective of the criss-crossing chains.

final R value of 0.055, while the other stuck at 0.16. Moreover, the first set gave a chemically satisfactory set of bond lengths and angles, while the second did not. The first solution is thus assumed to be the correct one. The corresponding parameters are given in Table 2, and the observed and calculated structure factors in Table 3. In addition to the 'unobserved' reflexions, 8

Table 2. Final parameters for $\gamma\text{-Ba}[\text{AlO(OH)}_2]_2$

Figures in brackets represent the estimated standard deviation corresponding to the least significant digit.

	x/a	Positional parameter			Isotropic temperature factor B_{iso}
		y/b	z/c		
Ba	0	0	0		1.05 (1)
Al	0.0860 (2)	0.3556 (3)	0.0519 (8)		0.46 (4)
O(1)	0.1307 (4)	0.194 (1)	0.017 (1)		0.3 (1)
O(2) (hydroxyl)	0.0022 (4)	0.305 (2)	0.114 (3)		1.1 (2)
O(3) (hydroxyl)	0.0831 (7)	0.474 (1)	0.835 (2)		1.0 (2)

reflexions where the agreement between F_o and F_c was poor were omitted from the final cycles of refinement. These corresponded mainly either to very weak reflexions at high angles, or to reflexions very close to c^* which the mechanical construction of the Y190 makes it difficult to measure accurately.

Description of the structure

Fig. 1 shows the structure viewed along \mathbf{c} . Each aluminum atom is surrounded tetrahedrally by four oxygen atoms. These tetrahedra share corners [O(1)] to form chains, and it is assumed that the two unshared corners [O(2) and O(3)] correspond to hydroxyl groups. The temperature factors (Table 2) are in accordance with this assumption.

The barium atoms lie on the twofold axes, and the chains lie along the *d*-glide planes perpendicular to \mathbf{a} . This means that the chains run diagonally across the cell, with alternate chains running in opposite directions (Figs. 1 and 2). We believe that this is the first chain structure in which the chains do not run parallel to one another. There is no hydrogen bonding between the chains.

Details of the coordination polyhedra about Al and Ba are given in Table 4. The barium atom is surrounded by eight oxygen atoms which form a very distorted cube (Fig. 1). The four independent distances [Table

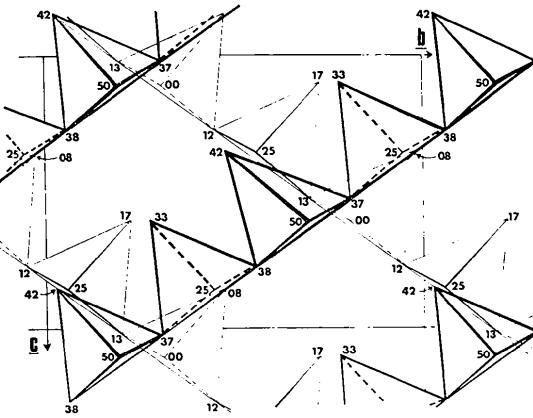


Fig. 2. The structure of $\gamma\text{-Ba}[\text{AlO(OH)}_2]_2$ viewed along \mathbf{a} , showing how the anion chains criss-cross. For simplicity only one half the unit cell, from 0 to $a/2$, is shown. Heights of oxygen atoms are expressed in $a/100$.

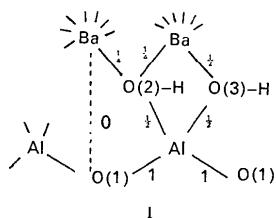
Table 3. Observed and calculated F values ($\times 10$)

Unobserved reflexions are marked with an asterisk.

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC					
** 2, x, 0	5.839	998	NH 2, x, 2	2, 1016	1468	NH 2, x, 2	2, 1020	1085	2, 1057	1089	2, 1058	1966	1, 1073	1101	NH 6, x, 8	5.1288	1150	6, 1233	63	NH 7, x, 10	7.025	642	8, 1059	967							
2 4174 4207			6 1283 1865	NH 5, x, 1	3, 3922	3543	0, 1151	1340	2, 1297	214	2, 2942	217	NH 19, x, 3	6, 1290	1553	5, 1132	1021	NH 7, x, 10	2, 1520	1548	4, 1588	1124	NH 12, x, 10	7.172	667	2, 0264	181	NH 7, x, 0			
NH 4, x, 0	1, 3451	3272	2, 1897	2051	4, 1879	1890	6, 1867	654	6, 3109	271	1, 1255	1355	8, 2700	281	7, 942	628	0, 2035	2884	0, 1524	1156	0, 1468	1364	3, 861	833	4, 332	23					
0 2716 2656	5 1950	2005	8 946	1280	8 1202	1729	5, 950	741	8, 680	1046	NH 16, x, 6	11, 1031	147	4, 1756	1730	3, 1601	1467	8, 686	935	2, 0581	3068	8, 293	58	5, 1223	1145	6, 1008	1059				
8 1789 1781	7 928	1004	NH 4, x, 2	NH 24, x, 2	5, 1046	1096	0, 2581	2667	1, 1071	147	6, 418	454	5, 961	919	NH 8, x, 8	5, 1804	1035	8, 987	885	7, 755	657	0, 1238	1183	1, 1501	1357	NH 4, x, 10	2, 2578	1152	1, 1591	1329	
NH 6, x, 0	5 3617	3505	2, 455	4242	2, 1081	1186	8, 3840	170	1, 1335	1475	6, 274	275	7, 987	969	4, 1845	1858	5, 996	912	0, 1554	2277	3, 1004	103	4, 1588	1530	5, 530	397	4, 655	1025			
2 3178 3037	3 1879	1890	6 2040	2155	6 2219	2216	6, 2017	2059	6, 1015	1129	5, 870	903	5, 964	978	NH 18, x, 4	1, 1061	1157	6, 418	454	5, 961	919	NH 8, x, 9	NH 8, x, 9	0, 1401	1401	0 348	92				
NH 8, x, 0	7 743	830	8 532	446	NH 26, x, 2	7 647	676	NH 21, x, 3	4, 1845	1858	5, 996	912	0, 2714	208	1, 1769	1008	4, 2638	60	5, 1091	1030	0, 2510	2277	3, 1004	103	8, 934	701	NH 11, x, 0	NH 16, x, 10			
0 4542 4267	4 2511	2527	1 2121	2091	0 2277	2251	2, 265	373	1, 1535	1405	6, 1018	989	5, 1044	1200	3, 1004	1030	0, 4602	462	1, 1298	1235	6, 280	368	5, 1175	1157	2, 2578	1152	1, 1591	1329			
8 1674	1798	5 1169	1640	5 1264	1254	4, 1627	183	5, 1748	3315	5, 976	1003	NH 15, x, 5	0, 2714	208	1, 1769	1008	4, 2638	60	5, 1091	1030	4, 1588	1530	5, 530	397	4, 655	1025					
NH 10, x, 0	7 1264	1254	6 1627	183	8 1061	1157	3, 2845	2603	NH 8, x, 2	7 647	676	NH 20, x, 6	1, 1036	1084	0, 2581	2631	3, 1029	1081	5, 1091	1030	0, 2510	2276	3, 1004	103	1, 1323	1229	0, 975	67	0, 348	92	
2 3371 3388	NH 11, x, 1	5 995	1003	NH 8, x, 2	7 671	817	0 3209	439	NH 23, x, 3	4, 2150	2083	6, 1436	1636	7, 870	901	NH 15, x, 5	0, 2714	208	1, 1769	1008	4, 2638	60	5, 1091	1030	NH 11, x, 0	NH 16, x, 10	2, 2578	1152	1, 1591	1329	
NH 15, x, 0	1, 1135	1159	NH 8, x, 2	7 671	817	0 3203	2000	0, 1504	1779	5 1074	1074	6, 1494	1580	7, 1031	1008	NH 14, x, 6	1, 1160	1141	4, 597	652	NH 15, x, 0	NH 1, x, 11	1, 1323	1229	0, 975	67	0, 348	92			
NH 12, x, 0	3, 1701	1750	0 3192	1541	NH 3, x, 3	4, 2150	2083	6, 1436	1636	7, 870	901	NH 17, x, 5	0, 2714	208	1, 1769	1008	4, 2638	60	5, 1091	1030	NH 12, x, 8	5 1127	1142	5, 548	109	7, 506	487				
4 4607 4750	5 1532	1557	2, 2725	2744	8 1700	1718	6, 446	2495	NH 19, x, 5	1, 1061	1157	5 1074	1074	6, 541	465	NH 14, x, 6	1, 1265	1251	3, 1029	2055	NH 15, x, 0	NH 5, x, 11	3, 1277	1173	1, 701	662	4, 350	211			
4 2016 1997	7 1063	1056	4, 1707	1786	5, 1533	1553	2, 1370	3087	NH 22, x, 4	8 702	819	1, 165	714	5, 1114	1161	NH 21, x, 5	0, 2714	208	1, 1769	1008	4, 2638	60	5, 1091	1030	NH 14, x, 10	3, 1048	1156	3, 948	847	3, 1080	1156
8 807	718	NH 13, x, 1	8 445	465	5 1832	1859	8 1187	1202	7, 1132	1222	0, 704	704	5, 1046	1292	8 818	8 1263	1298	NH 15, x, 7	0, 2097	2244	NH 15, x, 9	8 1263	1298	1, 1289	1257	1, 1403	1414				
NH 14, x, 0	3, 1410	1409	NH 10, x, 2	NH 5, x, 3	3 1105	1065	0, 2541	2521	0, 3044	3197	0, 3247	3210	0, 3045	3197	NH 11, x, 6	1, 1028	1078	3, 1029	2055	0, 975	67	0, 348	92	2, 2058	1251	1, 1591	1329				
2 2778 2019	3 1602	1513	0 2800	2872	NH 5, x, 3	2, 1103	1073	1, 1831	1850	8 3049	2014	4, 3374	337	NH 21, x, 5	0, 2714	208	1, 1769	1008	4, 2638	60	5, 1091	1030	0, 2081	2276	3, 1004	103	2, 2578	1152	1, 1591	1329	
8 1607	1624	7 997	1004	4, 2152	2207	1, 1611	1520	6, 1173	1273	NH 23, x, 5	8 329	173	NH 24, x, 4	3 261	2492	3 2040	2774	1, 1188	1321	5, 981	980	4, 1872	1889	1, 906	1048	NH 3, x, 11	NH 5, x, 11				
NH 16, x, 0	NH 15, x, 1	NH 10, x, 2	NH 7, x, 3	2, 1067	885	8 306	294	NH 20, x, 6	1, 1036	1084	0, 2581	2631	3, 1220	1177	8 327	350	6, 1231	1266	3, 1120	1177	8 324	315	6, 316	225	5, 765	681					
0 2307	2203	1, 1728	1792	3 1601	1649	1, 1911	1748	0 3741	3007	NH 24, x, 4	1, 1036	1084	0, 2581	2631	3 2040	2774	1, 1188	1321	5, 981	980	4, 1872	1889	1, 906	1048	NH 3, x, 11	NH 5, x, 11					
4 1499	1589	3 1595	2123	NH 12, x, 2	7 1401	1377	5, 1048	1048	4 2009	2014	7 329	173	NH 22, x, 5	1, 1072	1124	3 2040	2774	1, 1188	1321	5, 981	980	4, 1872	1889	1, 906	1048	NH 3, x, 11	NH 5, x, 11				
NH 18, x, 0	5 931	946	7 1048	1108	0 396	449	1, 1911	1748	2 1067	885	5 3205	3133	NH 23, x, 5	1, 1065	1054	1, 1546	1706	NH 16, x, 8	6 1437	1387	0 506	881	1, 936	818	7 712	681					
2 1308 1349	NH 17, x, 1	4, 1537	247	3 1105	1065	8 1713	1007	NH 6, x, 4	1, 1026	1076	0 3204	2774	5 3190	3186	6 1257	1260	NH 15, x, 7	0, 2097	2244	NH 15, x, 9	0, 2097	2244	0 9491	1526	NH 9, x, 11	NH 11, x, 11					
6 1444	1430	1, 1595	2175	8 266	89	3 1250	2138	2 2041	2061	7 1239	1288	6, 1687	1648	8 333	269	1, 1593	1575	NH 18, x, 8	6 324	315	6 316	225	5, 765	681							
0 1676	1674	4, 1595	2185	5 1333	1356	6 1524	1553	NH 25, x, 5	5, 1134	1124	6, 1593	1575	NH 21, x, 7	8 376	321	6, 1231	1266	8 324	315	6, 316	225	5, 765	681								
4 1224	1239	2, 993	1125	5 1537	1543	8 214+	213	NH 2, x, 6	1, 1274	2197	0 3221	2132	6, 1687	1648	8 333	269	3 1258	1263	NH 20, x, 6	6 321	315	6, 316	225	5, 765	681						
8 999	1004	1, 1559	1730	4 1923	1909	5 1537	1543	NH 3, x, 3	1, 1274	2197	0 3221	2132	6, 1687	1648	8 333	269	3 1258	1263	NH 22, x, 6	6 323	315	6, 316	225	5, 765	681						
HZ 22, x, 0	3 1965	1925	0 1066	974	NH 11, x, 3	0 3276	3166	2 837	830	7 601	542	6, 558	554	8 1191	1042	6, 340	316	NH 21, x, 7	0 343	88	6, 322	317	6 322	317							
2 2167	2313	7 667	558	NH 11, x, 2	0 3259	3166	2 837	830	7 601	542	6, 558	554	8 1191	1042	6, 340	316	NH 20, x, 8	6 322	317	6, 322	317	6 322	317								
6 1014	1174	NH 21, x, 1	0 656	699	3 1182	1192	6, 2305	2350	NH 5, x, 5	8 1199	1121	1, 1279	1272	NH 6, x, 6	2, 1024	1076	0 354	277	2 1380	1500	6 757	544	NH 1, x, 12	NH 2, x, 12							
0 2269	2752	1, 1055	1135	4 530	546	5, 1202	1219	6, 2305	2350	NH 5, x, 5	8 1199	1121	1, 1279	1272	NH 6, x, 6	2, 1024	1076	0 354	277	2 1380	1500	6 757	544	NH 1, x, 12	NH 2, x, 12						
NH 26, x, 0	3 1262	1369	2 2049	2124	7 924	913	0 1199	1121	1, 1279	1272	NH 6, x, 6	2, 1024	1076	0 354	277	2 1380	1500	6 757	544	0 2501	2475	0 525	527	2 106	1120	2 1228	1188				
2 1003	1171	NH 25, x, 1	0 1706	795	2 495	385	7 901	910	0 1199	1121	1, 1279	1272	NH 6, x, 6	2, 1024	1076	0 354	277	2 1380	1500	6 757	544	0 2501	2475	0 525	527	2 106</					

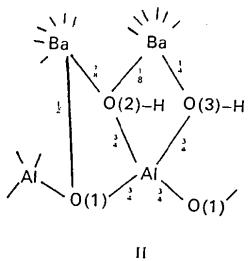
4(b)] vary from 2.77 to 3.03 Å. There are no other barium oxygen contacts below 3.2 Å, and for the purpose of applying Pauling's rules (see below) these longer contacts are assumed not to represent bonds. The Al-O tetrahedron is somewhat irregular, with the Al-O(2) bond significantly longer than the rest. A possible explanation of this is that this oxygen atom forms bonds to two barium atoms, and that this weakens the Al-O linkage. This can be illustrated by considering the different ways in which Pauling's rules can be applied to the structure:

(a) Assume that Al-O has bond order 1, and Al-OH bond order $\frac{1}{2}$. This leads to the following picture:



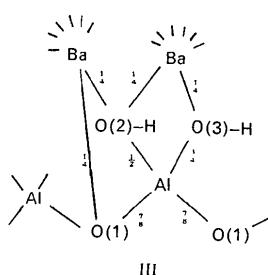
which is unsatisfactory on several counts, although it does explain why Ba-O(3) is shorter than either of the Ba-O(2) distances. However the enormous variation in bond order for the various Ba-O contacts is not supported by the distances listed in Table 4.

(b) Assume that all Al-O bonds are of equal order *i.e.* $\frac{3}{4}$. The picture is then:



This is again unsatisfactory, since it would suggest that Ba-O(1) should be the shortest contact.

(c) Assume that all Ba-O bonds are equal, *i.e.* of order $\frac{1}{4}$. This leads to:



and this is in many ways the most satisfactory picture. It explains the variation of Al-O bond lengths very neatly, although it does not account for the variations in Ba-O contacts.

Table 4. *Coordination polyhedra in γ -Ba[AlO(OH)₂]₂*

Figures in brackets give estimated standard deviations corresponding to the least significant digit.

(a) Al-O tetrahedron

	Bond distances
Al-O(1) (bridge)	1.74 (1) Å
Al-O(1') (bridge)	1.73 (1)
Al-O(2) (hydroxyl)	1.84 (1)
Al-O(3) (hydroxyl)	1.75 (1)
	Bond angles
O(1)-Al-O(1')	105.8 (5)°
O(1)-Al-O(2)	108.9 (6)
O(1)-Al-O(3)	115.1 (6)
O(1')-Al-O(2)	108.3 (6)°
O(1')-Al-O(3)	111.8 (5)
O(2)-Al-O(3)	106.8 (6)

(b) Ba-O coordination

Since the barium atoms lie on twofold axes, each contact occurs twice.

Ba-O(1')	2.930 (9) Å
Ba-O(2)	2.84 (2)
Ba-O(2')	3.03 (2)
Ba-O(3')	2.77 (1)

All of the above represent over-simplifications in one way or another, and the true situation presumably lies somewhere between these three assignments.

It is interesting to compare this structure with that of α -Ba[AlO(OH)₂]₂ (Ahmed & Dent Glasser, 1970), which also contains $[\text{AlO(OH)}_2]_\infty$ chains. In the α -modification the chains are kinked into an almost helical configuration, they run parallel to one another, and there is hydrogen bonding between the chains. It may well be that the γ -modification is difficult to prepare because the arrangement of chains in a criss-cross pattern is inherently less favoured than arrangement in a parallel one; the absence of hydrogen bonding and distortion of the Al-O tetrahedra may also betoken strain in the structure.

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