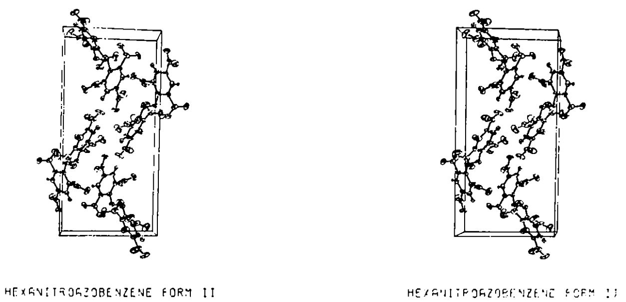

Fig. 7. Stereo pair illustrating the molecular packing in HNAB, form II.

whereas in form II they are rotated to each other by 81°. The center of symmetry in form I demands that the torsion angle about the azo linkage be 180°; this restriction is removed in form II and the angle becomes 177·5° which indicates a slight twist or strain in the double bond of the azo group. Furthermore, the angles between the carbon ring planes and the azo group (*i.e.*, plane through ring C(1) and C(1)–N=N in form II) are 49·4 and 50·9° for C(1) and C(11), respectively, compared with the single value of 43·2° in form I. These differences in the configurations and particularly the 81° twist of the planes result in less efficient molecular packing and is probably important in yielding the higher-energy less-stable form II polymorph with a lower (≈3%) density.

As seen in the stereo molecular packing illustrations of Fig. 7, the angle of rotation of the nitro groups seems to be dependent primarily upon steric effects. Even though the thermal motion for nitrogen and oxygen atoms is quite large, there appears to be no significant intermolecular interactions in the structure.

The authors are grateful to D. J. Gould for growing HNAB single crystals, R. A. Trudo for assistance in collecting intensity data, and A. C. Larson for not only providing 3D-Fourier plotting routines but also giving encouragement in the elucidation of the form II structure by direct methods.

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The Crystal Structure of $BaCd_{4 \cdot 43}$

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$BaCd_{4 \cdot 43}$ has a hexagonal sub-cell, space group *P*6/*mmm*, with lattice constants $a = 10{\cdot}740$ (3), $c = 10{\cdot}200$ (3) Å, $\varrho_{obs} = 7{\cdot}35$ g cm^{-3}. The true unit cell appears to be hexagonal with doubled *a* and *c* axes. A reasonable solution has been obtained for the sub-cell by the symbolic addition method using photographic data. The sub-cell contains 7 atoms of Ba and 31 of Cd, with one set of cadmium positions partially occupied.

In a previous paper (Bruzzone, 1972) a phase had been reported to exist in the Ba–Cd system with the approximate composition $BaCd_{4 \cdot 5}$ and a preliminary examination of a single crystal had shown hexagonal symmetry of Laue group 6/*mmm*. The purpose of the present work was the determination of the crystal structure of this phase.

Starting with Ba 99·5% pure supplied by Fluka (Switzerland) and Cd 99·999% pure produced by Koch-Light Co. (Great Britain), alloys of the composition $BaCd_{4 \cdot 5}$ were melted in iron crucibles under argon. After melting, some samples were quenched and some were annealed at 500°C.

Single-crystal techniques confirmed the Laue symmetry as $6/mmm$ and the lattice constants, subsequently refined from powder photographs were:

$$a = 10{\cdot}740 \pm 0{\cdot}003\ , \quad c = 10{\cdot}200 \pm 0{\cdot}003\ \text{Å}\ .$$

For all crystals examined, the rotation patterns around the x and z axes showed additional layer lines with very weak reflexions, which would double the a and c axes reported above. However, owing to the small number and weakness of these reflexions, the work was limited to the structural analysis of the sub-cell.

The intensity measurements were obtained from a well formed prismatic crystal elongated on the sixfold axis with dimensions of $1{\cdot}7 \times 0{\cdot}15 \times 0{\cdot}09$ mm. Integrated precession photographs, taken with Zr-filtered Mo radiation, provided 492 independent reflexions of which 286 observed reflexions were measured with a microdensitometer and 206 unobserved were assumed to have a value equal to one third of the least observable intensity, following the criterion of Hamilton (1955). The resulting data were corrected for Lorentz, polarization and absorption effects.

As no systematic absences were noted among the observed reflexions and the statistical analysis of the normalized structure factors gave a result closer to a centric distribution, the structure of the sub-cell was assumed to be centrosymmetric with the probable space group $P6/mmm$.

The symbolic addition procedure (Karle & Karle, 1966) was applied and a group of 81 phases determined. A three-dimensional Fourier map based on these 81 reflexions revealed 41 peaks of which seven could be ascribed to Ba atoms and the remainder to Cd atoms. In the simplifying assumption of the sub-cell all the interatomic distances were permissible save those between the six coplanar Cd atoms placed around the $0,0,\frac{1}{2}$ position, for which a half filling was taken.

A full-matrix least-squares refinement with isotropic thermal parameters yielded a final R value of 0·146 for the 286 observed reflexions.

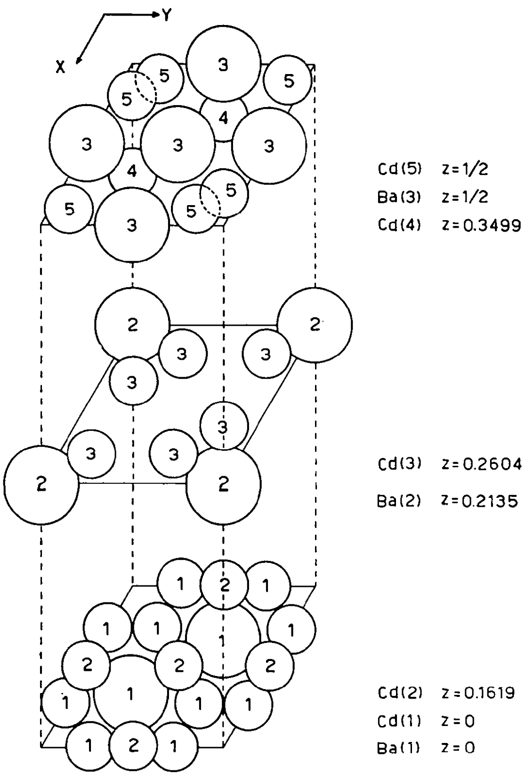

Fig. 1. Projection of the atoms onto the xy plane at various levels of z. Large circles Ba; small circles Cd.

Table 1. *Positional and thermal parameters of* $BaCd_{4.43}$

Space group $P6/mmm$, $\varrho_{obs} = 7{\cdot}35\ \text{g cm}^{-3}$, $\varrho_{cal} = 7{\cdot}25\ \text{g cm}^{-3}$
(Estimated standard deviations are given in parentheses.)

	Position	x	y	z	B(Å^2)
Ba(1)	2c	$\frac{1}{3}$	$\frac{2}{3}$	0	0·6 (3)
Ba(2)	2e	0	0	0·2135 (18)	0·9 (3)
Ba(3)	3g	$\frac{1}{2}$	0	$\frac{1}{2}$	2·0 (4)
Cd(1)	6j	0·2708 (11)	0	0	0·7 (2)
Cd(2)	6i	$\frac{1}{2}$	0	0·1619 (12)	1·2 (2)
Cd(3)	12o	0·1852 (4)	$-x$	0·2604 (8)	1·4 (2)
Cd(4)	4h	$\frac{1}{3}$	$\frac{2}{3}$	0·3499 (14)	1·1 (3)
Cd(5)	6m*	0·1038 (31)	$-x$	$\frac{1}{2}$	6.1 (9)

* The set Cd(5) has an occupancy factor of $\frac{1}{2}$.

Table 2. *Observed and calculated structure factors of* $BaCd_{4.43}$

(An asterisk indicates reflexions too weak for measurement.)

h	k	l		F_{obs}	F_{cal}
0	0	1		83.0	119.5
0	0	2		118.9	-145.0
0	0	3	*	39.2	42.7
0	0	4		749.9	755.9
0	0	5		120.0	122.3
0	0	6		355.8	350.2
0	0	7		147.5	180.1
0	0	8		529.5	549.4
0	0	9		184.0	-54.7
0	0	10	*	65.5	-51.5
0	0	11		169.0	270.9
0	0	12		535.1	559.2
0	0	13	*	19.4	2.6
0	0	14		244.7	142.2
1	0	2	*	20.4	-7.9
1	0	3		103.2	-59.0
1	0	4		193.6	193.6
1	0	5	*	47.9	47.6
1	0	6		96.6	-124.0
1	0	7		90.9	35.7
1	0	8	*	18.4	-7.4
1	0	9	*	63.5	71.6
1	0	10		121.7	90.8
1	0	11	*	30.0	-35.2
1	0	12	*	66.7	-75.7
1	1	1		95.1	-80.6
1	1	2	*	17.0	-1.0
1	1	3		191.5	175.0
1	1	4		212.1	-178.5
1	1	5		146.3	113.1
1	1	6		113.0	90.0
1	1	7		220.8	-219.8
1	1	8		101.8	-65.2
1	1	9		217.9	201.5
1	1	10	*	21.0	16.2
1	1	11	*	16.4	-11.7
1	1	12		118.6	-90.2
1	1	13	*	30.0	-23.2
1	1	14		170.3	-88.0
2	0	2	*	58.6	65.8
2	0	3		708.3	-647.6
2	0	4		220.1	-212.0
2	0	5	*	16.4	-2.5
2	0	6		261.9	260.6
2	0	7		156.7	-139.6
2	0	8		209.6	-182.3
2	0	9		194.4	-171.6
2	0	10	*	56.0	56.5
2	0	11		201.2	-182.3
2	0	12	*	30.0	-13.8
2	0	13	*	64.5	64.1
2	1	0		114.0	-61.9
2	1	1	*	16.4	-8.1
2	1	2		381.9	-405.1
2	1	3	*	40.8	-42.5
2	1	4		149.2	151.6
2	1	5	*	32.0	-31.2
2	1	6		399.3	-373.9
2	1	7	*	27.8	-24.9
2	1	8	*	29.8	-21.7
2	1	9	*	31.6	-26.4
2	1	10	*	34.0	-51.5
2	1	11	*	31.8	-32.5
2	1	12		102.1	-87.4
3	0	0		227.6	241.3
3	0	1		268.9	234.9
3	0	2		208.8	214.3
3	0	3		457.9	428.9
3	0	4	*	25.8	-32.5
3	0	5		311.6	344.7
3	0	6		235.1	260.0
3	0	7	*	33.6	-37.3
3	0	8	*	71.9	52.2
3	0	9		390.7	-353.8
3	0	10		152.8	144.4
3	0	11		132.1	98.1
3	0	12	*	16.0	1.8
3	0	13		88.4	81.1
2	2	0		1001.6	1020.1
2	2	1		70.8	-84.6
2	2	2		460.8	-476.6
2	2	3		138.0	-160.4
2	2	4		218.1	250.1
2	2	5	*	53.0	-47.4
2	2	6		106.9	80.3
2	2	7	*	16.0	-14.4
2	2	8		229.9	241.5
2	2	9		182.0	-181.3
2	2	10		157.8	-205.4
2	2	11		113.4	99.7
2	2	12		245.7	204.5
2	2	13		117.1	-97.5
3	1	0		150.2	-108.4
3	1	1		165.0	139.9
3	1	2		86.4	-40.1
3	1	3	*	41.7	47.6
3	1	4		123.4	108.6
3	1	5		157.0	129.7
3	1	6		146.3	-117.8
3	1	7	*	20.5	13.2
3	1	8	*	33.0	-29.6
3	1	9		147.9	131.1
3	1	10	*	75.0	97.7
3	1	11	*	35.6	-17.5
3	1	12	*	75.0	-72.4
4	0	0		339.9	329.0
4	0	1		204.1	263.6
4	0	2		242.2	250.7
4	0	3		263.4	-235.7
4	0	4		120.2	68.6
4	0	5		207.5	226.7
4	0	6		401.4	399.6
4	0	7	*	94.3	86.4
4	0	8	*	34.0	11.7
4	0	9	*	35.0	-6.7
4	0	10		211.8	177.8
4	0	11	*	30.0	-31.1
4	0	12		116.7	94.9
4	0	13		140.3	-161.7
3	2	0		309.5	-329.4
3	2	1		117.8	-80.6
3	2	2	*	35.4	-39.3
3	2	3		203.9	-152.1
3	2	4		92.8	-99.0
3	2	5	*	31.0	-20.6
3	2	6		140.5	-137.2
3	2	7		180.7	-161.7
3	2	8		175.6	-179.1
3	2	9	*	31.0	28.1
3	2	10		90.8	54.3
3	2	11		154.5	-130.4
3	2	12		170.4	-171.9
4	1	0		103.3	113.0
4	1	1	*	46.0	44.9
4	1	2		60.0	54.3
4	1	3		187.1	252.9
4	1	4	*	30.2	-48.0
4	1	5		149.8	179.4
4	1	6		151.1	129.4
4	1	7		155.1	-114.2
4	1	8	*	30.2	17.7
4	1	9		210.8	235.3
4	1	10	*	30.4	56.3
4	1	11	*	37.6	47.5
4	1	12	*	37.6	-31.5
5	0	0		194.9	147.3
5	0	1		98.6	8.7
5	0	2		337.9	-445.7
5	0	3		119.8	14.8
5	0	4		297.6	294.4
5	0	5		126.3	-43.9
5	0	6		374.6	405.2
5	0	7	*	32.2	42.8
5	0	8		144.7	84.7
5	0	9	*	30.0	-51.6
5	0	10	*	30.0	-85.2
5	0	11	*	30.0	28.3
5	0	12	*	32.2	-24.5
5	0	13		82.2	-83.0
3	3	0		284.8	267.6
3	3	1	*	47.9	-30.7
3	3	2	*	47.9	29.1
3	3	3		231.3	191.9
3	3	4	*	55.3	77.8
3	3	5		104.3	101.2
3	3	6		101.8	96.4
3	3	7		126.7	-135.3
3	3	8		108.2	82.8
3	3	9		206.1	182.5
3	3	10	*	33.4	29.5
3	3	11	*	31.8	61.1
3	3	12	*	27.6	-3.5
4	2	0		120.2	125.3
4	2	1	*	45.6	-76.4
4	2	2	*	45.6	52.4
4	2	3		533.1	-543.2
4	2	4		108.8	-94.0
4	2	5	*	54.6	-36.0
4	2	6		215.0	213.8
4	2	7		139.9	-119.0
4	2	8		127.8	-126.9
4	2	9		180.2	-160.4
4	2	10	*	66.9	41.4
4	2	11		174.7	-158.8
5	1	0		146.5	-154.1
5	1	1		103.4	-75.1
5	1	2		237.7	-273.1
5	1	3		150.4	-117.6
5	1	4		81.4	30.8
5	1	5		65.6	-63.2
5	1	6		265.6	-292.0
5	1	7		131.2	-92.6
5	1	8		70.6	-88.0
5	1	9	*	39.1	-30.1
5	1	10	*	41.2	-39.6
5	1	11	*	37.5	-81.4
5	1	12		176.0	-122.4
6	0	0		815.6	725.6
6	0	1	*	20.0	3.6
6	0	2		250.0	-261.6
6	0	3		127.0	-91.6
6	0	4		142.8	142.0
6	0	5	*	35.4	39.6
6	0	6		207.4	163.6
6	0	7	*	39.6	-4.0
6	0	8		221.2	176.6
6	0	9		88.6	-95.0
6	0	10		120.2	-121.2
6	0	11	*	90.7	84.7
6	0	12		194.2	173.0
4	3	0		274.8	290.8
4	3	1		121.4	84.0
4	3	2		178.0	-145.0
4	3	3		114.5	78.2
4	3	4		426.5	409.7
4	3	5	*	45.6	50.0
4	3	6		207.1	-190.0
4	3	7		95.4	101.4
4	3	8		170.1	170.5
4	3	9	*	49.7	42.2
4	3	10	*	49.7	35.6
4	3	11	*	49.7	70.2
4	3	12	*	45.6	37.4
5	2	0	*	26.2	-11.8
5	2	1	*	27.6	27.6
5	2	2	*	30.0	74.5
5	2	3		156.7	140.3
5	2	4		142.0	-139.5
5	2	5		149.8	120.8
5	2	6		155.1	129.0
5	2	7		156.8	-173.0
5	2	8	*	55.0	54.7
5	2	9		224.5	192.8
6	1	0		230.5	249.0
6	1	1	*	53.4	39.0
6	1	2	*	55.0	-3.2
6	1	3	*	56.5	-52.1
6	1	4	*	59.0	-57.1
6	1	5	*	61.0	69.2
6	1	6	*	64.8	-83.2
6	1	7	*	70.5	-75.1
6	1	8		164.7	-124.8
6	1	9		105.1	79.7
6	1	10	*	75.0	83.7
6	1	11	*	75.0	-84.3
6	1	12		158.2	-126.0
4	4	0		840.0	822.3
4	4	1		166.5	122.0
4	4	2	*	27.6	-7.4
4	4	3	*	29.2	23.2
4	4	4		233.1	269.7
4	4	5		201.2	157.2
4	4	6		294.9	330.3
4	4	7		109.0	86.3
4	4	8		233.9	260.0
4	4	9		32.4	17.7
4	4	10		20.4	3.2
4	4	11		131.0	150.6
4	4	12		266.2	234.5
7	0	0		151.7	-136.7
7	0	1		174.3	186.4
7	0	2		202.2	187.2
7	0	3		75.2	87.6
7	0	4	*	33.6	40.4
7	0	5		185.5	214.3
7	0	6		81.2	81.2
7	0	7	*	39.6	28.7
7	0	8	*	40.2	-42.1
7	0	9		200.7	196.1
7	0	10		170.6	195.3
5	3	0		186.5	-151.3
5	3	1	*	20.0	29.4
5	3	2	*	24.4	-4.0
5	3	3	*	25.4	-45.3
5	3	4	*	25.4	16.3
5	3	5		110.0	56.4
5	3	6		162.8	-83.4
5	3	7	*	61.4	-55.2
5	3	8		117.0	-77.0
5	3	9		119.7	70.3
5	3	10	*	66.0	78.2
5	3	11	*	66.9	-61.9
5	3	12		149.1	-99.3
6	2	0		115.2	119.5
6	2	1	*	55.9	-42.4
6	2	2		142.4	-110.0
6	2	3		386.6	-420.3
6	2	4	*	61.2	-64.3
6	2	5	*	61.7	-41.1
6	2	6	*	68.5	78.3
6	2	7	*	20.7	-73.9
6	2	8	*	72.0	-97.2
6	2	9		153.2	-180.3
7	1	0		223.1	201.0
7	1	1		149.3	92.6
7	1	2	*	24.8	-17.1
7	1	3		266.6	278.3
7	1	4		112.6	115.5
7	1	5		190.1	165.4
7	1	6	*	78.6	69.6
7	1	7	*	90.8	-9.2
7	1	8		85.2	123.3
7	1	9		226.4	200.8
7	1	10	*	72.6	30.1
7	1	11		125.5	111.0
5	4	0		249.0	-278.0
5	4	1	*	20.4	-6.4
5	4	2	*	25.6	2.4
5	4	3		111.4	-93.4
5	4	4		91.2	-104.8
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5	4	6	*	49.6	-75.6
5	4	7		130.0	-109.4
5	4	8		144.2	-190.1
5	4	9	*	49.6	58.6
5	4	10	*	49.8	71.4
5	4	11		93.1	-109.6
5	4	12		156.9	-143.9
6	3	0	*	21.0	12.0
6	3	1	*	31.0	-78.1
6	3	2	*	62.1	-50.1
6	3	3		131.4	130.3
6	3	4	*	67.1	-100.6
6	3	5	*	69.2	81.0
6	3	6	*	70.2	31.4
6	3	7		132.2	-139.9
6	3	8	*	74.3	-34.3
6	3	9		140.6	143.2
8	0	0		163.3	225.7
8	0	1		146.0	120.2
8	0	2		95.3	147.5
8	0	3		185.9	-253.6
8	0	4	*	33.6	40.4
8	0	5		146.4	120.3
8	0	6		197.6	272.1
8	0	7	*	37.2	33.6
8	0	8	*	30.0	-4.6
8	0	9	*	30.0	35.5
8	0	10		104.6	117.1
7	2	0		169.5	109.8
7	2	1		104.8	-54.8
7	2	2		365.9	-400.5
7	2	3	*	31.6	-39.0
7	2	4		239.0	221.5
7	2	5		104.8	-93.0
7	2	6		383.8	-351.0
8	1	0	*	34.0	-28.7
8	1	1	*	34.6	-33.1
8	1	2		179.9	-172.0
8	1	3	*	71.4	-61.7
8	1	4	*	73.6	97.9
8	1	5	*	37.8	-29.5
8	1	6		207.4	-204.2
8	1	7	*	30.2	-42.3
8	1	8	*	30.2	-20.6
8	1	9	*	30.2	-13.8
8	1	10	*	30.2	-12.6
8	1	11	*	34.0	-39.0
5	5	0		175.5	186.2
5	5	1	*	61.8	-55.3
5	5	2		218.0	-224.7
5	5	3		140.4	133.0
5	5	4	*	61.8	55.8
5	5	5	*	64.8	13.3
5	5	6	*	64.8	-100.2
5	5	7	*	64.8	-86.3
5	5	8	*	61.8	64.5
5	5	9	*	59.6	40.3
5	5	10		139.3	-85.3
6	4	0		102.2	177.4
6	4	1	*	29.8	21.8
6	4	2	*	79.8	-30.5
6	4	3		251.9	-314.2
7	3	0	*	63.7	-85.0
7	3	1	*	63.7	69.7
7	3	2	*	66.1	-10.8
7	3	3	*	66.1	8.9
7	3	4	*	65.5	51.6
7	3	5	*	70.7	79.3
9	0	0	*	30.0	-9.3
9	0	1	*	30.0	-37.6
9	0	2		70.1	87.6
9	0	3		74.5	89.4
9	0	4		104.5	-112.4
9	0	5		74.5	88.8
9	0	6		123.4	124.3
9	0	7		157.5	-156.7
9	0	8	*	30.1	-40.9
9	0	9		109.9	163.2
9	0	10		85.9	52.0
8	2	0		420.0	416.1
8	2	1	*	20.3	-16.5
8	2	2		83.5	-81.4
8	2	3		94.5	-112.0
8	2	4	*	40.0	6.9
8	2	5	*	44.8	42.0
8	2	6		211.1	204.9
6	5	0		88.3	66.5
6	5	1	*	24.8	-30.6
6	5	2		204.4	-235.8
6	5	3	*	24.8	-26.5
6	5	4		166.1	170.0
6	5	5	*	25.0	-38.5
6	5	6		230.7	-245.5
9	1	0		184.7	-214.8
9	1	1	*	68.0	-64.5
9	1	2	*	69.2	-29.1
9	1	3		120.2	-128.5
9	1	4	*	71.7	-78.2
9	1	5	*	72.9	-20.8
9	1	6	*	74.3	-95.4
9	1	7		122.6	-124.4
9	1	8		120.9	-137.0
9	1	9	*	32.4	14.0
9	1	10	*	34.0	36.8
9	1	11		117.1	-111.8
7	4	0		186.8	190.0
7	4	1		184.5	152.8
7	4	2		184.4	196.8
7	4	3		191.4	206.4
7	4	4	*	36.0	44.0
7	4	5		184.5	239.8
7	4	6		246.0	226.8
7	4	7	*	32.8	1.5
7	4	8	*	45.0	78.1
7	4	9		274.3	268.6
8	3	0	*	61.5	-77.5
8	3	1		91.5	104.8
8	3	2		115.4	87.2
8	3	3	*	64.3	35.5
8	3	4	*	66.9	47.8
8	3	5		107.4	121.8
8	3	6	*	69.5	13.3
10	0	0		183.3	280.2
10	0	1	*	24.4	10.0
10	0	2		124.9	-85.1
10	0	3		191.3	-253.0
10	0	4		124.9	117.6
10	0	5	*	24.4	-8.2
6	6	0		214.7	314.0
6	6	1	*	64.8	-52.3
6	6	2	*	64.8	-57.3
6	6	3		134.8	-141.8
6	6	4		96.6	-41.5
6	6	5	*	61.8	14.6
6	6	6		164.1	188.0
7	5	0		138.8	-141.4
10	1	0		180.3	191.2
10	1	1	*	36.2	32.6
10	1	2	*	36.2	-14.5
10	1	3		145.5	172.6
10	1	4	*	45.3	82.0
8	4	0		201.6	257.1
8	4	1	*	70.7	70.3
8	4	2	*	70.7	-63.2
8	4	3		173.9	-186.4
9	3	0		198.1	214.7
9	3	1	*	21.6	-7.9
9	3	2		197.0	-161.0
9	3	3		153.7	150.6
11	0	0		225.5	254.9
11	0	1		106.6	109.8
11	0	2		124.4	-122.2
11	0	3		105.8	114.1
11	0	4		296.7	326.7
11	0	5	*	69.7	64.4
7	6	0		99.9	-153.6
7	6	1	*	52.7	-39.4
7	6	2	*	52.7	-21.9
7	6	3	*	52.7	-92.1
7	6	4	*	52.7	-43.4
9	4	0	*	49.5	42.9
9	4	1	*	49.5	-42.6
9	4	2		244.3	-248.7
9	4	3	*	49.5	-47.3
9	4	4		132.3	127.9
9	4	5	*	51.9	-61.2
9	4	6		237.6	-248.0
12	0	0		236.3	299.9
12	0	1	*	69.7	67.2
12	0	2	*	67.2	59.6
7	7	0		296.7	337.2
7	7	1	*	55.6	67.4
7	7	2		73.2	-86.8
7	7	3		192.0	214.8
7	7	4		176.4	200.4
7	7	5		71.5	93.6
8	7	0	*	61.2	85.5
8	7	1	*	55.9	73.4
8	7	2	*	55.2	-35.7
8	7	3	*	55.0	53.5
8	7	4		147.1	157.8

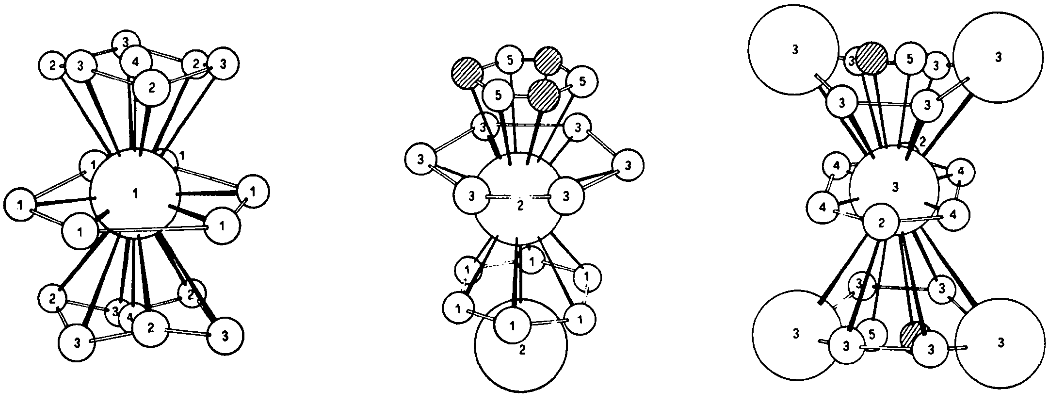

Fig. 2. Coordination around the Ba atoms. Large circles Ba; small circles Cd. The set Cd(5) is partially occupied and the shaded circles are missing atoms.

Table 3. *Interatomic distances in* $BaCd_{4\cdot43}$ (Å)

Ba(1)	6 Cd(1)	3·96
	6 Cd(2)	3·51
	6 Cd(3)	3·83
	2 Cd(4)	3·57
Ba(2)	1 Ba(2)	4·36
	6 Cd(1)	3·63
	6 Cd(3)	3·48
	*6 Cd(5)	3·50
Ba(3)	4 Ba(3)	5·37
	2 Cd(2)	3·45
	8 Cd(3)	3·83
	4 Cd(4)	3·46
	*4 Cd(5)	3·82
Cd(1)	2 Ba(1)	3·96
	2 Ba(2)	3·63
	2 Cd(1)	2·91
	2 Cd(2)	2·97
	4 Cd(3)	3·17
Cd(2)	2 Ba(1)	3·51
	1 Ba(3)	3·45
	2 Cd(1)	2·97
	1 Cd(2)	3·30
	4 Cd(3)	3·11
	2 Cd(4)	3·65
Cd(3)	1 Ba(1)	3,83
	1 Ba(2)	3·48
	2 Ba(3)	3·83
	2 Cd(1)	3·17
	2 Cd(2)	3·11
	2 Cd(3)	3·45
	1 Cd(4)	2·90
	*1 Cd(5)	2·88
	*2 Cd(5)	3·86
Cd(4)	1 Ba(1)	3·57
	3 Ba(3)	3·46
	3 Cd(2)	3·65
	3 Cd(3)	2·90
	1 Cd(4)	3·06
Cd(5)	2 Ba(2)	3·50
	2 Ba(3)	3·82
	2 Cd(3)	2·88
	4 Cd(3)	3·86
	*2 Cd(5)	3·35
	*1 Cd(5)	3·86
	*2 Cd(5)	1·93

* The multiplicity of bonds marked with an asterisk is dependent on the degree of occupancy of the Cd(5) set.

The final parameters for the sub-cell of $BaCd_{4\cdot43}$ are given in Table 1; observed and calculated structure factors are shown in Table 2. The reflexions 100, 101, 110, 200 and 201 could not be recorded by the precession method and are omitted from the list.

In Fig. 1 projections of the atoms onto the *xy* plane at various levels of *z* from $z=0$ to $z=\frac{1}{2}$ are shown.

Interatomic distances are given in Table 3 and are not unusual, except for the Cd(5)–Cd(5) distance between atoms in adjacent sites, which is too small (1·93 Å) to permit simultaneous occupancy. Placing the atoms in alternate sites results in acceptable values (3·35 Å).

The coordination around each type of atom was evaluated using the atomic distribution gap criterion described elsewhere (Bruzzone, Fornasini & Merlo, 1970). The average coordination numbers of the Ba and Cd atoms are 18·9 and 12·1, respectively. The arrangements of the atoms around every crystallographic type of Ba are drawn in Fig. 2 and are somewhat similar: Ba(1) and Ba(3) both have 20 neighbours, but Ba(1) is surrounded by Cd atoms only, while Ba(3) is surrounded by four Ba atoms and 16 Cd atoms. The lower coordination number (16) for Ba(2) is due to the one-half filling of the Cd(5) set; moreover, Ba(2) has only one Ba(2) atom at a distance of 4·36 Å instead of a pair of Ba atoms. It should be noted that the polyhedra about the Ba atoms show some resemblance to those of the larger atom in the $CaZn_5$ structure type.

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