Obviously, the slit itself may be regarded as a source, when its dimension $a \simeq \lambda$. However, such a condition is never satisfied for X-rays. In this connection a consistent analysis of the slit role in forming the interference pattern, with an account of source–crystal–film distance, is of interest.

References

AFANAS'EV, A. M. & KOHN, V. G. (1977). *Fiz. Tverd. Tela*, **19**, 1775–1783.

ARISTOV, V. V. & POLOVINKINA, V. I. (1978). *Acta Cryst.* A**34**, S227.

ARISTOV, V. V., POLOVINKINA, V. I., SHMYT'KO, I. M. & SKULAKOV, E. V. (1978). *Pis'ma Zh. Eksp. Teor. Fiz.* **28**, 6–9.

BORN, H. & WOLF, E. (1964). *Principles of Optics*. New York: Pergamon Press.

EWALD, P. P. (1917). *Ann. Phys.* **54**, 519–597.

HART, M. & MILNE, A. D. (1968). *Phys. Status Solidi*, **26**, 185–189.

JEFFREYS, H. & SWIRLES, B. (1966). *Method of Mathematical Physics*. Cambridge Univ. Press.

KATO, N. (1961). *Acta Cryst.* **14**, 526–533, 627–636.

KATO, N. (1968). *J. Appl. Phys.* **39**, 2225–2230, 2231–2237.

KATO, N. & LANG, A. R. (1959). *Acta Cryst.* **12**, 787–794.

KOHN, V. G. (1979). *Kristallografiya*, **24**, 712–719.

KOZMIK, V. D. & MIKHAILYUK, I. P. (1978). *Ukr. Fiz. Zh.* (*Ukr. Ed.*), **23**, 1570–1571.

PINSKER, Z. G. (1978). *Dynamical Scattering of X-rays in Perfect Crystals*. Heidelberg, London, New York: Springer Verlag.

Acta Cryst. (1980). A**36**, 1013–1016

Restrictions in the Arrangement of Molecular Sheets in CdI_2 and PbI_2 Polytypes

BY M. A. WAHAB AND G. C. TRIGUNAYAT

Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India

(*Received* 30 *January* 1980; *accepted* 5 *June* 1980)

Abstract

Based on the observations that in the Zhdanov symbols of the known CdI_2 and PbI_2 structures the occurrence of number 3 is far less frequent than the occurrence of numbers 1 and 2 and numbers greater than 3 do not occur at all, a review of these structures has been made. Empirical rules have been evolved, which help in drastically cutting down the number of possible structures of a given polytype and thus considerably facilitate the process of its crystal-structure determination.

Introduction

The layered compounds CdI_2 and PbI_2 are known to be rich in polytypism. Over 260 polytypes of the former and 50 polytypes of the latter have been reported, of which the crystal structures of 90 and 15, respectively, have been determined. An examination of the known structures, listed in Tables 1 and 2, reveals that their Zhdanov symbols rarely contain the number 3. This has led to the formulation of a useful empirical guideline, using which the number of probable structures for a given polytype is drastically reduced.

0567-7394/80/061013-04$01.00

The nature of the arrangement of molecular sandwiches in the known structures of CdI_2 and PbI_2

The analysis of the structures of CdI_2 and PbI_2 crystals (Tables 1 and 2), grown by various techniques (from solution, melt, vapour and gel) and numbering 105 in all, shows that they are made up of combinations of different types of molecular sandwiches, with each sandwich consisting of a sheet of cadmium atoms nested between two sheets of iodine atoms. All sandwiches are geometrically equivalent but can have six possible orientations, with three belonging to a cyclic group, *viz* $A\gamma B$, $B\alpha C$ and $C\beta A$ and three to an anticyclic group, *viz* $B\gamma A$, $C\alpha B$ and $A\beta C$. The smallest polytype $2H$ is formed by a periodic repetition of any of the above six sandwiches. The second smallest polytype $4H$ ($A\gamma B$ $C\alpha B$ ...) contains sandwiches from alternate groups. The higher polytypes consist of various combinations of sandwiches from the two groups.

Out of the crystal structures listed in Tables 1 and 2, the existence of three structures, *viz* $6H_2$ and $32H_1$ of CdI_2 and $6R$ of PbI_2, is doubtful for the following reasons. (*a*) Although the polytypes $6H_2$ and $6R$ have been reported by Pinsker & co-workers (Pinsker, 1941; Pinsker, Tatarinova & Novikova, 1943), and the poly-

Table 1. *Stacking sequences of* CdI_2 *polytypes with known crystal structure*

The structures marked with *, † and ‡ have been reported by Min & Ohsumi (1976), Jain & Trigunayat (1978) and Jain, Wahab & Trigunayat (1978), respectively. The rest have been taken from a recent review (Trigunayat & Verma, 1976).

	Polytype	Zhdanov symbol	Stacking sequence
1	$2H$	11	$A\gamma B \ldots$
2	$4H$	22	$A\gamma B\ C\alpha B \ldots$
3	$6H_1$	2211	$A\gamma B\ C\alpha B\ A\gamma B \ldots$
4	$6H_2$	33	$A\gamma B\ C\beta A\ C\alpha B$
5	$8H_1$	$22(11)_2$	$A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B$
6	$8H_2$	$(121)_2$	$A\gamma B\ A\beta C\ A\beta C\ A\gamma B$
7	$8H_3$	1232	$A\gamma B\ A\beta C\ A\gamma B\ C\alpha B$
8	$10H_1$	$(22)_2 11$	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B$
9	$10H_2$	$(221)_2$	$A\gamma B\ C\alpha B\ A\gamma B\ A\beta C\ A\gamma B$
10	$10H_3$	$22(11)_3$	$A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B\ A\gamma B$
11	$10H_4$	$2(11)_2 211$	$A\gamma B\ C\alpha B\ C\alpha B\ C\alpha B\ A\gamma B$
12	$12H_1$	222123	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ C\beta A\ C\alpha B$
13	$12H_2$	$(21)_2(12)_2$	$A\gamma B\ C\alpha B\ C\beta A\ C\beta A\ C\alpha B\ C\alpha B$
14	$12H_3$	$(22)_2(11)_2$	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B$
15	$12H_4$	$22(211)_2$	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ C\alpha B\ A\gamma B$
16	$12H_5$	11123211	$A\gamma B\ A\gamma B\ A\beta C\ A\gamma B\ C\alpha B\ A\gamma B$
17	$12H_6$	22111221	$A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B\ A\beta C\ A\gamma B$
18	$12H_7$	$22(11)_4$	$A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B\ A\gamma B\ A\gamma B$
19	$12H_8$	$22112(11)_3$	$A\gamma B\ C\alpha B\ C\alpha B\ A\gamma B\ A\gamma B\ A\gamma B$
20	$12R$	$(13)_3$	$A\gamma B\ A\beta C\ B\alpha C\ B\gamma A\ C\beta A\ C\alpha B$
21	$14H_1$	$(22)_3 11$	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B$
22	$14H_2$	$(1122)_2 11$	$A\gamma B\ A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B\ C\alpha B\ A\gamma B$
23	$14H_3$	11212322	$A\gamma B\ A\gamma B\ C\alpha B\ C\beta A\ C\alpha B\ A\gamma B\ C\alpha B$
24	$14H_4$	$(22)_2(11)_3$	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B\ A\gamma B$
25	$14H_5$	$2112(11)_4$†	$A\gamma B\ C\alpha B\ C\alpha B\ A\gamma B\ A\gamma B\ A\gamma B\ A\gamma B$
26	$16H_1$	$(22)_2(211)_2$	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ C\alpha B\ A\gamma B$
27	$16H_2$	$(22)_2(11)_4$	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B\ A\gamma B\ A\gamma B$
28	$16H_3$	$22(212)_2 11$	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ C\beta A\ C\alpha B\ C\alpha B\ A\gamma B$
29	$16H_4$	$(22)_3(11)_2$	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B$
30	$16H_5$	12223222	$A\gamma B\ A\beta C\ A\gamma B\ A\beta C\ A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B$
31	$16H_6$	$(22)_2 112211$	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B\ C\alpha B\ A\gamma B$
32	$16H_7$	$1232(22)_2$	$A\gamma B\ A\beta C\ A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B$
33	$16H_8$	$(22211)_2$†	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B$
34	$18H_1$	$(22)_4 11$	$(A\gamma B\ C\alpha B)_4\ A\gamma B$
35	$18H_2$	$22(11)_7$	$A\gamma B\ C\alpha B\ (A\gamma B)_7$
36	$18H_3$	1222322211	$A\gamma B\ A\beta C\ A\gamma B\ A\beta C\ A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ A\gamma B$
37	$18H_4$	$22(212)_2(11)_2$	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ C\beta A\ C\alpha B\ C\alpha B\ A\gamma B\ A\gamma B$
38	$18H_5$	$(22)_3 1221$	$(A\gamma B\ C\alpha B)_3\ A\gamma B\ A\beta C\ A\gamma B$
39	$18H_6$	$2(2211)_2 211$‡	$A\gamma B\ C\alpha B\ A\gamma B\ C\alpha B\ C\alpha B\ A\gamma B\ C\alpha B\ C\alpha B\ A\gamma B$
40	$18R_1$	$(2121)_3$†	$A\gamma B\ C\alpha B\ C\beta A\ C\beta A\ B\gamma A\ B\alpha C\ B\alpha C\ A\beta C\ A\gamma B$
41	$20H_1$	$(22)_4(11)_2$	$(A\gamma B\ C\alpha B)_4\ A\gamma B\ A\gamma B$
42	$20H_2$	$22(11)_2(2112)_2$	$A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B\ A\gamma B\ C\alpha B\ C\alpha B\ A\gamma B\ C\alpha B\ C\alpha B$
43	$20H_3$	$22(11)_8$	$A\gamma B\ C\alpha B\ (A\gamma B)_8$
44	$20H_4$	$(11)_7 2112$	$(A\gamma B)_7\ A\gamma B\ C\alpha B\ C\alpha B$
45	$20H_5$	$(22)_2 21122211$	$(A\gamma B\ C\alpha B)_3\ (C\alpha B\ A\gamma B)_2$
46	$20H_6$	$(22)_3(211)_2$	$(A\gamma B\ C\alpha B)_4\ C\alpha B\ A\gamma B$
47	$20H_7$	$(221111)_2 1111$†	$(A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B)_2\ A\gamma B\ A\gamma B$
48	$20H_8$	$(22)_3 112211$†	$(A\gamma B\ C\alpha B)_3\ A\gamma B\ A\gamma B\ C\alpha B\ A\gamma B$
49	$20H_9$	$(11)_5 211222$*	$(A\gamma B)_6\ (C\alpha B)_2\ A\gamma B\ C\alpha B$
50	$22H_1$	$(11)_5(2211)_2$	$(A\gamma B)_5\ (A\gamma B\ C\alpha B\ A\gamma B)_2$
51	$22H_2$	$(22)_2 2112(11)_4$‡	$(A\gamma B\ C\alpha B)_3\ C\alpha B\ (A\gamma B)_4$
52	$22H_3$	$(22)_2 11(22)_2(11)_2$‡	$(A\gamma B\ C\alpha B)_2\ A\gamma B\ (A\gamma B\ C\alpha B)_2\ A\gamma B\ A\gamma B$
53	$24H_1$	$(2222211)_2$	$(A\gamma B\ C\alpha B)_3\ C\alpha B\ (A\gamma B\ C\alpha B)_2\ A\gamma B$
54	$24H_2$	$2221(22)_3 23$	$(A\gamma B\ C\alpha B)_2\ (C\beta A\ C\alpha B)_4$
55	$24H_3$	$(22)_4 12211$†	$(A\gamma B\ C\alpha B)_4\ A\gamma B\ A\gamma B\ C\alpha B\ A\gamma B$
56	$24H_4$	$(2211)_2 1122(11)_3$†	$(A\gamma B\ C\alpha B\ A\gamma B)_2\ A\gamma B\ A\gamma B\ C\alpha B\ (A\gamma B)_3$
57	$24H_5$	$(22)_2 1122(11)_2 2211$†	$(A\gamma B\ C\alpha B)_2\ A\gamma B\ A\gamma B\ C\alpha B\ (A\gamma B)_3\ C\alpha B\ A\gamma B$
58	$24H_6$	$(211)_3 112221111$†	$A\gamma B\ C\alpha B\ C\alpha B\ (A\gamma B)_2\ (C\alpha B)_3\ A\gamma B\ C\alpha B\ A\gamma B\ A\gamma B$
59	$24H_7$	$222112(22)_2(11)_3$‡	$(A\gamma B\ C\alpha B)_2\ C\alpha B\ (A\gamma B\ C\alpha B)_2\ (A\gamma B)_3$
60	$24R_1$	$(2213)_3$	$A\gamma B\ C\alpha B\ A\gamma B\ (A\beta C\ B\alpha C)_2\ (B\gamma A\ C\beta A)_2\ C\alpha B$
61	$24R_2$	$(212111)_3$†	$A\gamma B\ C\alpha B\ (C\beta A)_3\ B\gamma A\ (B\alpha C)_3\ A\beta C\ A\gamma B\ A\gamma B$
62	$26H_1$	$(21111)_4 11$	$A\gamma B\ (C\alpha B)_3\ (A\gamma B)_3\ (C\alpha B)_3\ (A\gamma B)_3$
63	$26H_2$	$(22)_6 11$	$(A\gamma B\ C\alpha B)_6\ A\gamma B$

Table 1 (*cont.*)

	Polytype	Zhdanov symbol	Stacking sequence
64	$26H_3$	$(222211)_2 2112$	$(A\gamma B~C\alpha B~A\gamma B~C\alpha B~A\gamma B)_2~A\gamma B~C\alpha B~C\alpha B$
65	$28H_1$	$(22)_6(11)_2$	$(A\gamma B~C\alpha B)_6~A\gamma B~A\gamma B$
66	$28H_2$	$(22)_4 11(22)_2 11$	$(A\gamma B~C\alpha B)_4~A\gamma B~(A\gamma B~C\alpha B)_2~A\gamma B$
67	$28H_3$	$(22)_5 112211$	$(A\gamma B~C\alpha B)_5~A\gamma B~A\gamma B~C\alpha B~A\gamma B$
68	$28H_4$	$(22)_2(11)_4 22(11)_4$	$(A\gamma B~C\alpha B)_2~(A\gamma B)_4~A\gamma B~C\alpha B~(A\gamma B)_4$
69	$28H_5$	$(22)_2 2(11)_2 22(11)_4$‡	$(A\gamma B~C\alpha B)_3~(C\alpha B)_2~A\gamma B~C\alpha B~(A\gamma B)_4$
70	$30H_1$	$(2211)_4 1122$	$(A\gamma B~C\alpha B~A\gamma B)_4~A\gamma B~A\gamma B~C\alpha B$
71	$30H_2$	$(22)_2(211)_2(22)_3 11$	$(A\gamma B~C\alpha B)_3~C\alpha B~A\gamma B~(A\gamma B~C\alpha B)_3~A\gamma B$
72	$30H_3$	$(22)_7 11$	$(A\gamma B~C\alpha B)_7~A\gamma B$
73	$30H_4$	$(22)_4 211222(11)_2$	$(A\gamma B~C\alpha B)_5~C\alpha B~A\gamma B~C\alpha B~A\gamma B~A\gamma B$
74	$30H_5$	$(22)_2 2112211(22)_2 211$‡	$(A\gamma B~C\alpha B)_3~C\alpha B~A\gamma B~C\alpha B~C\alpha B~(A\gamma B~C\alpha B)_2~A\gamma B$
75	$30R_1$	$(221212)_3$	$A\gamma B~C\alpha B~A\gamma B~A\beta C~(A\beta C~B\alpha C)_2~B\gamma A~(B\gamma A~C\beta A)_2~C\alpha B~C\alpha B$
76	$30R_2$	$(21211111)_3$†	$A\gamma B~C\alpha B~(C\beta A)_4~B\gamma A~(B\alpha C)_4~A\beta C~(A\gamma B)_3$
77	$32H_1$	$(22)_5 321123$	$(A\gamma B~C\alpha B)_5~A\gamma B~C\beta A~C\alpha B~C\alpha B~C\beta A~C\alpha B$
78	$34H_1$	$(222211)_3 22$	$(A\gamma B~C\alpha B~A\gamma B~C\alpha B~A\gamma B)_3~A\gamma B~C\alpha B$
79	$36H_1$	$(22221111)_2(11)_2(22)_2$	$(A\gamma B~C\alpha B)_2~(A\gamma B)_2~(A\gamma B~C\alpha B)_2~(A\gamma B)_4~(A\gamma B~C\alpha B)_2$
80	$36R_1$	$(22112121)_3$	$A\gamma B~C\alpha B~(A\gamma B)_2~C\alpha B~(C\beta A)_2~B\gamma A~(C\beta A)_2~B\gamma A~(B\alpha C)_2~A\beta C~(B\alpha C)_2~A\beta C~(A\gamma B)_2$
81	$36R_2$	$(22212111)_3$	$(A\gamma B~C\alpha B)_2~C\beta A~C\alpha B~(C\beta A~B\gamma A)_2~(B\alpha C)_2~(B\alpha C~A\beta C)_2~(A\gamma B)_2$
82	$36R_3$	$(22211121)_3$‡	$(A\gamma B~C\alpha B)_2~C\alpha B~C\beta A~(C\beta A~B\gamma A)_2~B\gamma A~(B\alpha C)_2~A\beta C~B\alpha C~(A\beta C)_2~A\gamma B$
83	$36R_4$	$(221223)_3$‡	$A\gamma B~C\alpha B~(A\gamma B~A\beta C)_2~B\alpha C~A\beta C~(B\alpha C~B\gamma A)_2~C\beta A~B\gamma A~(C\beta A~C\alpha B)_2$
84	$38H_1$	$(22)_9 11$	$(A\gamma B~C\alpha B)_9~A\gamma B$
85	$40H_1$	$(22)_7 21122211$	$(A\gamma B~C\alpha B)_7~A\gamma B~C\alpha B~C\alpha B~A\gamma B~C\alpha B~A\gamma B$
86	$42R_1$	$(22221212)_3$	$(A\gamma B~C\alpha B)_2~A\gamma B~(A\beta C)_2~(B\alpha C~A\beta C)_2~B\alpha C~(B\gamma A)_2~(C\beta A~B\gamma A)_2~C\beta A~(C\alpha B)_2$
87	$60R_1$	$[(22)_3 1223]_3$	$(A\gamma B~C\alpha B)_3~(A\gamma B~A\beta C)_2~(B\alpha C~A\beta C)_3~(B\alpha C~B\gamma A)_2~(C\beta A~B\gamma A)_3~(C\beta A~C\alpha B)_2$
88	$72R_1$	$[(22)_4 1223]_3$	$(A\gamma B~C\alpha B)_4~(A\gamma B~A\beta C)_2~(B\alpha C~A\beta C)_4~(B\alpha C~B\gamma A)_2~(C\beta A~B\gamma A)_4~(C\beta A~C\alpha B)_2$
89	$84R_1$	$[(22)_5 211121]_3$	$(A\gamma B~C\alpha B)_5~A\gamma B~C\alpha B~C\alpha B~C\beta A~(C\beta A~B\gamma A)_5~C\beta A~B\gamma A~B\gamma A~B\alpha C~(B\alpha C~A\beta C)_5~B\alpha C~A\beta C~A\beta C~A\gamma B$
90	$84R_2$	$[(22)_5 121211]_3$	$(A\gamma B~C\alpha B)_5~A\gamma B~(A\beta C)_2~B\alpha C~(B\alpha C~A\beta C)_5~B\alpha C~(B\gamma A)_2~C\beta A~(C\beta A~B\gamma A)_5~C\beta A~(C\alpha B)_2~A\gamma B$

type $6R$ has also been reported by Hanoka & Vand (1968), it is remarkable that none of the subsequent workers (*e.g.* Trigunayat & Verma, 1976; Jain & Trigunayat, 1979), who have investigated thousands of CdI_2 and PbI_2 crystals by single-crystal methods, have encountered any of these polytypes, which casts serious doubts about their actual existence. Neither Pinsker *et al.* nor Hanoka & Vand have reproduced the diffraction photographs of these structures. Besides, the investigations of Pinsker *et al.* were made by electron diffraction in the early forties, when the technique had not been well perfected. (*b*) The CdI_2 polytype $32H_1$ has been reported by Prasad & Srivastava (1970). However, it has been pointed out that the observed intensities on their published X-ray diffraction photographs do not tally with the calculated values and therefore the reported structure determination is wrong (Jain & Wahab, 1979). Hence it can be concluded that this structure does not really exist, according to the information available so far. Excluding these three polytypes from Tables 1 and 2 and examining the stacking sequences of the rest of the polytypes, we observe the following characteristic feature:

Table 2. *Stacking sequences of* PbI_2 *polytypes with known structures*

The structures marked with *, † and ‡ have been reported by Minagawa (1979), Chand & Trigunayat (1976) and Chand (1976), respectively. The rest have been taken from a recent review (Trigunayat & Verma, 1976).

	Polytype	Zhdanov symbol	*ABC* sequence
1	$2H$	11	$A\gamma B \ldots$
2	$4H$	22	$A\gamma B~C\alpha B \ldots$
3	$6H$	2211	$A\gamma B~C\alpha B~A\gamma B \ldots$
4	$6R$		$A\gamma B~C\beta A~B\alpha C \ldots$
5	$8H$	1232*	$A\gamma B~A\beta C~A\gamma B~C\alpha B$
6	$10H$	$(11)_3 22$	$(A\gamma B)_3~A\gamma B~C\alpha B$
7	$10H_2$	$11(112)_2$*	$(A\gamma B)_3~(C\alpha B)_2$
8	$10H_3$	$11(22)_2$*	$A\gamma B~(A\gamma B~C\alpha B)_2$
9	$12R_1$	$(13)_3$	$A\gamma B~A\beta C~B\alpha C~B\gamma A~C\beta A~C\alpha B$
10	$14H_1$	$(11)_6 22$	$(A\gamma B)_6~A\gamma B~C\alpha B$
11	$20H_1$	$(11)_7 2112$	$(A\gamma B)_7~A\gamma B~C\alpha B~C\alpha B$
12	$22H$	$11(22)_5$*	$A\gamma B~(A\gamma B~C\alpha B)_5$
13	$24H_1$	$(11)_5(211)_3 2$†	$(A\gamma B)_6~(C\alpha B)_2~(A\gamma B)_2~(C\alpha B)_2$
14	$24H_2$	$(11)_4(211)_2(112)_2$‡	$(A\gamma B)_5~(C\alpha B)_2~(A\gamma B)_3~(C\alpha B)_2$
15	$30R$	$(111313)_3$*	$(A\gamma B)_2~A\beta C~B\alpha C~B\gamma A~(C\beta A)_2~C\alpha B~A\gamma B~A\beta C~(B\alpha C)_2~B\gamma A~C\beta A~C\alpha B$

The different molecular sandwiches belonging to a group do not exist in succession in the stacking sequence of a given polytype.

For instance, consider the stacking sequence of the polytype $8H_2$, *viz* $|A\gamma B~A\beta C~A\beta C~A\gamma B|~A\gamma B~A\beta C \ldots$. Focusing attention on the second sandwich $A\beta C$ and considering the possibility of its being succeeded by another sandwich from the anticyclic group, *viz* $B\gamma A$,

$C\alpha B$ or $A\beta C$, we find that the next sandwich is $A\beta C$ itself. The same holds for the sandwich $A\gamma B$, belonging to the cyclic group. Thus, two or more sandwiches of a group when occurring in succession in a structure, have essentially the same composition of layers.

Structure conditions for the formation of CdI_2 and PbI_2 polytypes

A geometrical condition for the formation of any MX_2 structure is that the different numbers of layers occurring in cyclic (n_+) and anticyclic (n_-) succession should be equal to 6γ for hexagonal structures and equal to $6\gamma \pm 2$ for rhombohedral structures, where γ is an integer (Verma & Krishna, 1966), *i.e.*

(1) $$n_+ + n_- = 6\gamma \text{ (hexagonal)}$$
$$= 6\gamma \pm 2 \text{ (rhombohedral)}.$$

In addition, the following empirical conditions exist regarding the occurrence of the known CdI_2 and PbI_2 polytypes.

(2) All numbers greater than 3 in the Zhdanov symbol are absent (see Tables 1 and 2).

(3) The cubicities of the structures are limited to 50% (Ram, 1974).

(4) The number 3 in the Zhdanov symbol occurs only after an odd sum of numbers.

Table 3. *Possible crystal structures of* CdI_2 *polytypes*

Polytype	Number of possibilities worked out earlier	Number of reduced possibilities	Known structures (see Table 1)	Undetermined structures
2*H*	1	1	11	–
4*H*	1	1	22	–
6*H*	2	1	2211	–
8*H*	8	3	$22(11)_2$, $(121)_2$ & 1232	–
10*H*	22	6	$(22)_2 11$, $(221)_2$, $22(11)_3$ & $2(11)_2 211$	212311 & 211123
12*H*	66	14	222123, $(21)_2(12)_2$ $(22)_2(11)_2$, $22(211)_2$, 11123211, 22111221, $22(11)_4$ & $22112(11)_3$	$(2111)_2$, $(221)_2 11$, $(213)_2$, 21231111, 21112311 & 21211311
6*R*	1	–	–	–
12*R*	2	1	$(13)_3$	–
18*R*	6	2	$(2121)_3$	$(1311)_3$
24*R*	14	4	$(2213)_3$ & $(212111)_3$	$(211121)_3$ & $(131111)_3$
30*R*	44	10	$(2211212)_3$ & $(21211111)_3$	$(21112111)_3$, $(221113)_3$, $(21111121)_3$, $(213211)_3$, $(13111111)_3$, $(221311)_3$, $(213121)_3$ & $(131311)_3$
36*R*	131	24	$(22112121)_3$, $(2212111)_3$, $(22211121)_3$ & $(221223)_3$	$(2121111111)_3$, $(2111211111)_3$, $(2111112111)_3$, $(2111111121)_3$, $(22121211)_3$, $(221313)_3$, $(213123)_3$, $(212313)_3$, $(22111113)_3$, $(22131111)_3$, $(21321111)_3$, $(22111311)_3$, $(21121113)_3$, $(21312111)_3$, $(21112131)_3$, $(21311211)_3$, $(21311121)_3$, $(222213)_3$, $(1311111111)_3$ & $(13131111)_3$.

These conditions are obtainable by analysing the Zhdanov symbols alone of the polytypes listed in Tables 1 and 2. However, conditions 2 and 4 also follow from the empirical rule established by us earlier, regarding the mode of stacking sequences of molecular sandwiches. Similarly, the condition 3 can also be deduced from the ABC sequences of the polytypes. This is only natural, since the ABC notation and Zhdanov symbol are just two different ways of describing the crystal structure of a given polytype and the one is directly convertible into the other. The above three empirical conditions drastically reduce the number of possible structures for a given polytype and thus greatly help in the process of its crystal-structure determination. Without applying these conditions, the total number of distinct possibilities for close-packed MX_2 compounds for hexagonal polytypes up to 12*H* and rhombohedral polytypes up to 36*R* were worked out earlier (*e.g.* Jain, 1976; Jain & Trigunayat, 1977), as shown in the second column of Table 3. The reduced numbers of possible structures obtained by employing the conditions are listed in the next column. Some of them have already been reported and have been listed in the fourth column. The structures that remain to be discovered and worked out are given in the last column. In a similar manner, with help from Table 2, a list of the known and unknown crystal structures of PbI_2 can be prepared.

References

CHAND, M. (1976). PhD Thesis. Delhi Univ.

CHAND, M. & TRIGUNAYAT, G. C. (1976). *J. Cryst. Growth*, **39**, 299–304.

HANOKA, J. I. & VAND, V. (1968). *J. Appl. Phys.* **39**, 5288–5297.

JAIN, P. C. (1976). PhD Thesis. Delhi Univ.

JAIN, P. C. & TRIGUNAYAT, G. C. (1977). *Acta Cryst.* A**33**, 257–260.

JAIN, P. C. & TRIGUNAYAT, G. C. (1978). *Acta Cryst.* B**34**, 2677–2684.

JAIN, P. C. & TRIGUNAYAT, G. C. (1979). *J. Cryst. Growth*. In the press.

JAIN, P. C. & WAHAB, M. A. (1979). Personal communication.

JAIN, P. C., WAHAB, M. A. & TRIGUNAYAT, G. C. (1978). *Acta Cryst.* B**34**, 2685–2690.

MIN, E. & OHSUMI, K. (1976). *Mineral. J.* **8**, 151–157.

MINAGAWA, T. (1979). *J. Appl. Cryst.* **12**, 57–59.

PINSKER, Z. G. (1941). *Acta Physicochim. URSS*, **14**, 530.

PINSKER, Z. G., TATARINOVA, L. & NOVIKOVA, V. (1943). *Acta Physicochim. URSS*, **18**, 378–386.

PRASAD, R. & SRIVASTAVA, O. N. (1970). *Z. Kristallogr.* **131**, 376–384.

RAM, U. S. (1974). *Phys. Status Solidi*, **23**, 197–208.

TRIGUNAYAT, G. C. & VERMA, A. R. (1976). *Physics and Chemistry of Materials with Layered Structures*, Vol. 2, edited by F. LEVY, pp. 286–288. Dordrecht: Reidel.

VERMA, A. R. & KRISHNA, P. (1966). *Polymorphism and Polytypes in Crystals*. New York: John Wiley.