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	作成者: Hosoya, Masahiko, 細谷, 将彦
	メールアドレス:
	所属:
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Corrected Summary of Crystal-Structure Types Enumerated by Computer

Masahiko Hosoya*

*Department of Physics and Earth Sciences, Faculty of Science, University of the Ryukyus, Nishihara, Okinawa 903-0213, Japan

Abstract

The enumeration of crystal-structure types in a previous paper [M. Hosoya: Bull. Faculty of Science, Univ. of the Ryukyus, 44 (1987) 11-74] is revised. Three types were found to be redundant in Genus A3B3. The computer program which was used in the enumeration and presented in another paper [M. Hosoya & K. Takushi: Bull. Faculty of Science, Univ. of the Ryukyus, 47 (1989) 23-71] is debugged.

Conclusion

Recently the Author's previous enumeration of crystal-structure types1)-6) was reassured in several papers of Fadda and Zanzotto7)-9). However some erroneous results were also found which originates in the computer program used10)-11). Fadda12) translated our BASIC program into one by FORTRAN and found that the following three species in Genus A3B3 are redundant.

Cm(8)_13:ab2aaa I4mmm(107)_6:ab2aaa P6mm(183)_6:ab2aaa

He pointed out that each is equivalent to Cm(8)_13:aaaab2, I4mmm(107)_6:aaaab2, and P6mm(183)_6:aaaab2, respectively. With his indication, the program10) was examined closely and its defective part was found. The following four lines should be put instead of the original ones. (Line 30255 is an additional one.)

11420 DATA -2,-2,-3,1, 0

21120 DATA -2,-2,-6,-2,-2,-2,-2,1,1, 0

30250 B(KA) = B(KA-NL%(MG)) : IF D%(B(KA)) = 0 THEN B(KA) = B(KA) + 1:GOTO 30260

30255 KB=KB+1: KA=KA+1: IF KB<=NL%(MG) THEN 30250 ELSE 30480

This revision adds P-421c(114)_3:a2d4 in Genus A6 and P-421c(114)_3:a2d4 in Genus A2B4.

Then the corrected summary of enumeration is given as follows.

Family	Genus	Species	
1	Α	14	
2	A2	29	
2	AB	51	
3	A3	114	

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^{*}Retired in 2006. Present address: Syuri-Kinzyoutyou 3-40-2, Naha-si, Okinawa 903-0815, Japan

3	AB2		125
3	ABC		44
4	A4		366
4	A2B2		296
4	AB3		244
4	ABC2		234
4	ABCD		64
5	A5		374
5	A2B3		680
5	AB4		530
5	AB2C2		500
5	ABC3		369
5	ABCD2	237	
5	ABCDE	52	
6	A6		1142 (Revised from the wrong value 1141)
6	A3B3		887 (Revised from the wrong value 890)
6	A2B4		2102 (Revised from the wrong value 2101)
6	A2B2C2	910	
6	AB5		958
6	AB2C3		1921
6	ABC4		986
6	ABC2D2	975	
6	ABCD3	476	
6	ABCDE2	313	
6	ABCDEF	69	

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