



FOUNDATIONS
ADVANCES

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Supporting information for article:

Normally supportive sublattices of crystallographic space groups

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1 Normally-supportive sublattices

Table S1: A table of normally supportive sublattices of crystallographic space groups, or rather of their arithmetic crystal classes (ACCs), according to cpg-normal subgroup. The first column contains the ACC number and representative symmorphic-space group symbol. The second column contains the name of the cpg-normal subgroup P_N and an integer index that identifies it in our data files and algorithms for a specific ACC. The third column is the HNF matrix B_N containing the column basis of the normally supportive sublattice, laid out row by row. These matrices are also accompanied by an integer index for convenience. The fourth column contains a case number (c#) that specifies a set of extra conditions from table S2 that the parameters in B_N must satisfy. When no case number is provided, the variables in B_N can take on any non-negative integer values.

ACC	P_N	B_N matrix row by row	c#
2 $\bar{1}P$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	9 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	12 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	13 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	14 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	15 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
2 $\bar{1}P$	2 $\bar{1}$	16 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
3 $2P$	2 2_y	1 $\{\{1, 0, 0\}, \{1 + c_1, 2 + 2c_1, 0\}, \{0, 0, 1\}\}$	
3 $2P$	2 2_y	2 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
3 $2P$	2 2_y	3 $\{\{1, 0, 0\}, \{1 + c_1, 2 + 2c_1, 0\}, \{1, 0, 2\}\}$	
3 $2P$	2 2_y	4 $\{\{1, 0, 0\}, \{1 + c_1, 2 + 2c_1, 0\}, \{0, 0, 2\}\}$	
3 $2P$	2 2_y	5 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1, 0, 2\}\}$	
3 $2P$	2 2_y	6 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1, 1, 2\}\}$	
3 $2P$	2 2_y	7 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 2\}\}$	
3 $2P$	2 2_y	8 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 1, 2\}\}$	
3 $2P$	2 2_y	9 $\{\{2, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
3 $2P$	2 2_y	10 $\{\{2, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 2\}\}$	
3 $2P$	2 2_y	11 $\{\{2, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 1, 2\}\}$	
4 $2C$	2 2_y	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
4 $2C$	2 2_y	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 2\}\}$	
4 $2C$	2 2_y	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 1, 2\}\}$	
5 mP	2 m_y	1 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{2c_2, 1 + c_2 + c_3, 2 + 2c_2 + 2c_3\}\}$	
5 mP	2 m_y	2 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + 2c_2, 1 + c_2 + c_3, 2 + 2c_2 + 2c_3\}\}$	
5 mP	2 m_y	3 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{2c_2, 0, 2 + 2c_2 + 2c_3\}\}$	
5 mP	2 m_y	4 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{2c_2, 0, 1 + 2c_2 + 2c_3\}\}$	
5 mP	2 m_y	5 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + 2c_2, 0, 2 + 2c_2 + 2c_3\}\}$	
5 mP	2 m_y	6 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + 2c_2, 0, 3 + 2c_2 + 2c_3\}\}$	
5 mP	2 m_y	7 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{c_2, 0, 1 + c_2 + c_3\}\}$	
5 mP	2 m_y	8 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{c_2, 0, 1 + c_2 + c_3\}\}$	
6 mC	2 m_y	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
6 mC	2 m_y	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_2, 2 + c_1 + c_2\}\}$	
6 mC	2 m_y	3 $\{\{1, 0, 0\}, \{1, 2 + c_3, 0\}, \{0, c_1, 1 + c_1 + c_2\}\}$	
7 $2/mP$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
7 $2/mP$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
7 $2/mP$	2 $\bar{1}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
7 $2/mP$	2 $\bar{1}$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
7 $2/mP$	2 $\bar{1}$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
7 $2/mP$	2 $\bar{1}$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
7 $2/mP$	2 $\bar{1}$	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
7 $2/mP$	2 $\bar{1}$	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
7 $2/mP$	2 $\bar{1}$	9 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
7 $2/mP$	2 $\bar{1}$	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
7 $2/mP$	2 $\bar{1}$	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
7 $2/mP$	2 $\bar{1}$	12 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
7 $2/mP$	2 $\bar{1}$	13 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
7 $2/mP$	2 $\bar{1}$	14 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
7 $2/mP$	2 $\bar{1}$	15 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
7 $2/mP$	2 $\bar{1}$	16 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
7 $2/mP$	3 2_y	1 $\{\{1, 0, 0\}, \{1 + c_1, 2 + 2c_1, 0\}, \{0, 0, 1\}\}$	
7 $2/mP$	3 2_y	2 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 1\}\}$	

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Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
7 2/mP	3 2 _y	3 {{1, 0, 0}, {1 + c ₁ , 2 + 2c ₁ , 0}, {1, 0, 2}}	
7 2/mP	3 2 _y	4 {{1, 0, 0}, {1 + c ₁ , 2 + 2c ₁ , 0}, {0, 0, 2}}	
7 2/mP	3 2 _y	5 {{1, 0, 0}, {0, 1 + c ₁ , 0}, {1, 0, 2}}	
7 2/mP	3 2 _y	6 {{1, 0, 0}, {0, 1 + c ₁ , 0}, {1, 1, 2}}	
7 2/mP	3 2 _y	7 {{1, 0, 0}, {0, 1 + c ₁ , 0}, {0, 0, 2}}	
7 2/mP	3 2 _y	8 {{1, 0, 0}, {0, 1 + c ₁ , 0}, {0, 1, 2}}	
7 2/mP	3 2 _y	9 {{2, 0, 0}, {0, 1 + c ₁ , 0}, {0, 0, 1}}	
7 2/mP	3 2 _y	10 {{2, 0, 0}, {0, 1 + c ₁ , 0}, {0, 0, 2}}	
7 2/mP	3 2 _y	11 {{2, 0, 0}, {0, 1 + c ₁ , 0}, {0, 1, 2}}	
7 2/mP	4 m _y	1 {{1 + c ₁ , 0, 0}, {0, 1, 0}, {2c ₂ , 1 + c ₂ + c ₃ , 2 + 2c ₂ + 2c _{3}}}	
7 2/mP	4 m _y	2 {{1 + c ₁ , 0, 0}, {0, 1, 0}, {1 + 2c ₂ , 1 + c ₂ + c ₃ , 2 + 2c ₂ + 2c _{3}}}	
7 2/mP	4 m _y	3 {{1 + c ₁ , 0, 0}, {0, 1, 0}, {2c ₂ , 0, 2 + 2c ₂ + 2c _{3}}}	
7 2/mP	4 m _y	4 {{1 + c ₁ , 0, 0}, {0, 1, 0}, {2c ₂ , 0, 1 + 2c ₂ + 2c _{3}}}	
7 2/mP	4 m _y	5 {{1 + c ₁ , 0, 0}, {0, 1, 0}, {1 + 2c ₂ , 0, 2 + 2c ₂ + 2c _{3}}}	
7 2/mP	4 m _y	6 {{1 + c ₁ , 0, 0}, {0, 1, 0}, {1 + 2c ₂ , 0, 3 + 2c ₂ + 2c _{3}}}	
7 2/mP	4 m _y	7 {{1 + c ₁ , 0, 0}, {0, 2, 0}, {c ₂ , 0, 1 + c ₂ + c _{3}}}	
7 2/mP	4 m _y	8 {{1 + c ₁ , 0, 0}, {1, 2, 0}, {c ₂ , 0, 1 + c ₂ + c _{3}}}	
7 2/mP	5 2/m _y	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
7 2/mP	5 2/m _y	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
7 2/mP	5 2/m _y	3 {{1, 0, 0}, {0, 1, 0}, {1, 0, 2}}	
7 2/mP	5 2/m _y	4 {{1, 0, 0}, {0, 1, 0}, {0, 1, 2}}	
7 2/mP	5 2/m _y	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
7 2/mP	5 2/m _y	6 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
7 2/mP	5 2/m _y	7 {{1, 0, 0}, {0, 2, 0}, {0, 0, 1}}	
7 2/mP	5 2/m _y	8 {{1, 0, 0}, {1, 2, 0}, {1, 0, 2}}	
7 2/mP	5 2/m _y	9 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
7 2/mP	5 2/m _y	10 {{1, 0, 0}, {0, 2, 0}, {1, 0, 2}}	
7 2/mP	5 2/m _y	11 {{1, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
7 2/mP	5 2/m _y	12 {{2, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
7 2/mP	5 2/m _y	13 {{2, 0, 0}, {0, 1, 0}, {0, 1, 2}}	
7 2/mP	5 2/m _y	14 {{2, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
7 2/mP	5 2/m _y	15 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1}}	
7 2/mP	5 2/m _y	16 {{2, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
8 2/mC	2 1	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
8 2/mC	2 1	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
8 2/mC	2 1	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
8 2/mC	2 1	4 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
8 2/mC	2 1	5 {{1, 0, 0}, {1, 2, 0}, {1, 0, 2}}	
8 2/mC	2 1	6 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
8 2/mC	2 1	7 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1}}	
8 2/mC	2 1	8 {{2, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
8 2/mC	3 2 _y	1 {{1, 0, 0}, {c ₁ , 1 + c ₁ , 0}, {0, 0, 1}}	
8 2/mC	3 2 _y	2 {{1, 0, 0}, {c ₁ , 1 + c ₁ , 0}, {0, 0, 2}}	
8 2/mC	3 2 _y	3 {{1, 0, 0}, {c ₁ , 1 + c ₁ , 0}, {1, 1, 2}}	
8 2/mC	4 m _y	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
8 2/mC	4 m _y	2 {{1, 0, 0}, {0, 1, 0}, {1 + c ₁ , 1 + c ₂ , 2 + c ₁ + c _{2}}}	
8 2/mC	4 m _y	3 {{1, 0, 0}, {1, 2 + c ₃ , 0}, {0, c ₁ , 1 + c ₁ + c _{2}}}	
8 2/mC	5 2/m _y	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
8 2/mC	5 2/m _y	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
8 2/mC	5 2/m _y	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
8 2/mC	5 2/m _y	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
8 2/mC	5 2/m _y	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
9 222P	2 2 _x	1 {{1 + c ₁ , 0, 0}, {0, 1, 0}, {0, 0, 1}}	
9 222P	2 2 _x	2 {{1 + c ₁ , 0, 0}, {0, 1, 0}, {0, 1, 2}}	
9 222P	2 2 _x	3 {{1 + c ₁ , 0, 0}, {0, 1, 0}, {1, 1, 2}}	
9 222P	2 2 _x	4 {{1 + c ₁ , 0, 0}, {0, 1, 0}, {0, 0, 2}}	
9 222P	2 2 _x	5 {{1 + c ₁ , 0, 0}, {0, 1, 0}, {1, 0, 2}}	
9 222P	2 2 _x	6 {{1 + c ₁ , 0, 0}, {0, 2, 0}, {0, 0, 1}}	
9 222P	2 2 _x	7 {{1 + c ₁ , 0, 0}, {1, 2, 0}, {0, 0, 1}}	
9 222P	2 2 _x	8 {{1 + c ₁ , 0, 0}, {0, 2, 0}, {0, 0, 2}}	
9 222P	2 2 _x	9 {{1 + c ₁ , 0, 0}, {0, 2, 0}, {1, 0, 2}}	
9 222P	2 2 _x	10 {{1 + c ₁ , 0, 0}, {1, 2, 0}, {0, 0, 2}}	
9 222P	2 2 _x	11 {{1 + c ₁ , 0, 0}, {1, 2, 0}, {1, 0, 2}}	
9 222P	3 2 _y	1 {{1, 0, 0}, {1 + c ₁ , 2 + 2c ₁ , 0}, {0, 0, 1}}	
9 222P	3 2 _y	2 {{1, 0, 0}, {0, 1 + c ₁ , 0}, {0, 0, 1}}	
9 222P	3 2 _y	3 {{1, 0, 0}, {1 + c ₁ , 2 + 2c ₁ , 0}, {1, 0, 2}}	
9 222P	3 2 _y	4 {{1, 0, 0}, {1 + c ₁ , 2 + 2c ₁ , 0}, {0, 0, 2}}	
9 222P	3 2 _y	5 {{1, 0, 0}, {0, 1 + c ₁ , 0}, {1, 0, 2}}	
9 222P	3 2 _y	6 {{1, 0, 0}, {0, 1 + c ₁ , 0}, {1, 1, 2}}	
9 222P	3 2 _y	7 {{1, 0, 0}, {0, 1 + c ₁ , 0}, {0, 0, 2}}	
9 222P	3 2 _y	8 {{1, 0, 0}, {0, 1 + c ₁ , 0}, {0, 1, 2}}	
9 222P	3 2 _y	9 {{2, 0, 0}, {0, 1 + c ₁ , 0}, {0, 0, 1}}	
9 222P	3 2 _y	10 {{2, 0, 0}, {0, 1 + c ₁ , 0}, {0, 0, 2}}	
9 222P	3 2 _y	11 {{2, 0, 0}, {0, 1 + c ₁ , 0}, {0, 1, 2}}	
9 222P	4 2 _z	1 {{1, 0, 0}, {0, 1, 0}, {1 + c ₁ , 1 + c ₁ , 2 + 2c _{1}}}	
9 222P	4 2 _z	2 {{1, 0, 0}, {0, 1, 0}, {1 + c ₁ , 0, 2 + 2c _{1}}}	
9 222P	4 2 _z	3 {{1, 0, 0}, {0, 1, 0}, {0, 1 + c ₁ , 2 + 2c _{1}}}	

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Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
9 222P	4 2 _z	4 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
9 222P	4 2 _z	5 {{1, 0, 0}, {1, 2, 0}, {1 + c ₁ , 0, 2 + 2c _{1}}}	
9 222P	4 2 _z	6 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c _{1}}}	
9 222P	4 2 _z	7 {{1, 0, 0}, {0, 2, 0}, {1 + c ₁ , 0, 2 + 2c _{1}}}	
9 222P	4 2 _z	8 {{1, 0, 0}, {0, 2, 0}, {0, 0, 1 + c _{1}}}	
9 222P	4 2 _z	9 {{2, 0, 0}, {0, 1, 0}, {0, 1 + c ₁ , 2 + 2c _{1}}}	
9 222P	4 2 _z	10 {{2, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
9 222P	4 2 _z	11 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1 + c _{1}}}	
9 222P	5 222	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
9 222P	5 222	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
9 222P	5 222	3 {{1, 0, 0}, {0, 1, 0}, {1, 0, 2}}	
9 222P	5 222	4 {{1, 0, 0}, {0, 1, 0}, {0, 1, 2}}	
9 222P	5 222	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
9 222P	5 222	6 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
9 222P	5 222	7 {{1, 0, 0}, {0, 2, 0}, {0, 0, 1}}	
9 222P	5 222	8 {{1, 0, 0}, {1, 2, 0}, {1, 0, 2}}	
9 222P	5 222	9 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
9 222P	5 222	10 {{1, 0, 0}, {0, 2, 0}, {1, 0, 2}}	
9 222P	5 222	11 {{1, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
9 222P	5 222	12 {{2, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
9 222P	5 222	13 {{2, 0, 0}, {0, 1, 0}, {0, 1, 2}}	
9 222P	5 222	14 {{2, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
9 222P	5 222	15 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1}}	
9 222P	5 222	16 {{2, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
10 222C	2 2 _x	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
10 222C	2 2 _x	2 {{1, 0, 0}, {1, 2 + c ₁ , 0}, {0, 0, 1}}	
10 222C	2 2 _x	3 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
10 222C	2 2 _x	4 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
10 222C	2 2 _x	5 {{1, 0, 0}, {1, 2 + c ₁ , 0}, {0, 0, 2}}	
10 222C	2 2 _x	6 {{1, 0, 0}, {1, 2 + c ₁ , 0}, {0, 1, 2}}	
10 222C	3 2 _y	1 {{1, 0, 0}, {c ₁ , 1 + c ₁ , 0}, {0, 0, 1}}	
10 222C	3 2 _y	2 {{1, 0, 0}, {c ₁ , 1 + c ₁ , 0}, {0, 0, 2}}	
10 222C	3 2 _y	3 {{1, 0, 0}, {c ₁ , 1 + c ₁ , 0}, {1, 1, 2}}	
10 222C	4 2 _z	1 {{1, 0, 0}, {0, 1, 0}, {1 + c ₁ , 1 + c ₁ , 2 + 2c _{1}}}	
10 222C	4 2 _z	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
10 222C	4 2 _z	3 {{1, 0, 0}, {1, 2, 0}, {1 + c ₁ , 0, 2 + 2c _{1}}}	
10 222C	4 2 _z	4 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c _{1}}}	
10 222C	4 2 _z	5 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1 + c _{1}}}	
10 222C	5 222	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
10 222C	5 222	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
10 222C	5 222	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
10 222C	5 222	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
10 222C	5 222	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
11 222F	2 2 _x	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
11 222F	2 2 _x	2 {{1, 0, 0}, {1, 2, 0}, {1 + c ₁ , c ₁ , 2 + c _{1}}}	
11 222F	2 2 _x	3 {{1, 0, 0}, {0, 1, 0}, {0, c ₁ , 1 + c _{1}}}	
11 222F	2 2 _x	4 {{1, 0, 0}, {0, 1, 0}, {1 + c ₁ , c ₁ , 2 + 2c _{1}}}	
11 222F	3 2 _y	1 {{1, 0, 0}, {1, 2, 0}, {c ₁ , 0, 1 + c _{1}}}	
11 222F	3 2 _y	2 {{1, 0, 0}, {0, 1, 0}, {c ₁ , 1 + c ₁ , 2 + 2c _{1}}}	
11 222F	3 2 _y	3 {{1, 0, 0}, {0, 1, 0}, {c ₁ , 0, 1 + c _{1}}}	
11 222F	4 2 _z	1 {{1, 0, 0}, {c ₁ , 1 + c ₁ , 0}, {1, 0, 2}}	
11 222F	4 2 _z	2 {{1, 0, 0}, {c ₁ , 1 + c ₁ , 0}, {0, 1, 2}}	
11 222F	4 2 _z	3 {{1, 0, 0}, {c ₁ , 1 + c ₁ , 0}, {0, 0, 1}}	
11 222F	5 222	1 {{1, 0, 0}, {0, 1, 0}, {0, 1, 2}}	
11 222F	5 222	2 {{1, 0, 0}, {0, 1, 0}, {1, 0, 2}}	
11 222F	5 222	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
11 222F	5 222	4 {{1, 0, 0}, {1, 2, 0}, {1, 0, 2}}	
11 222F	5 222	5 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
12 222I	2 2 _x	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
12 222I	2 2 _x	2 {{1, 0, 0}, {0, 1, 0}, {3 + 2c ₁ , 3 + 4c ₁ , 4(1 + c ₁)}}	
12 222I	2 2 _x	3 {{1, 0, 0}, {0, 1, 0}, {1, 1 + c ₁ , 2 + c _{1}}}	
12 222I	2 2 _x	4 {{2, 0, 0}, {0, 1, 0}, {0, 1, 2}}	
12 222I	2 2 _x	5 {{2, 0, 0}, {0, 1, 0}, {2, 3 + 2c ₁ , 2(2 + c ₁)}}	
12 222I	3 2 _y	1 {{1, 0, 0}, {0, 2, 0}, {1, 0, 2}}	
12 222I	3 2 _y	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
12 222I	3 2 _y	3 {{1, 0, 0}, {0, 2, 0}, {3 + 2c ₁ , 2, 2(2 + c ₁)}}	
12 222I	3 2 _y	4 {{1, 0, 0}, {0, 1, 0}, {3 + 4c ₁ , 3 + 2c ₁ , 4(1 + c ₁)}}	
12 222I	3 2 _y	5 {{1, 0, 0}, {0, 1, 0}, {1 + c ₁ , 1, 2 + c _{1}}}	
12 222I	4 2 _z	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
12 222I	4 2 _z	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
12 222I	4 2 _z	3 {{1, 0, 0}, {1, 2, 0}, {2, 2, 2(2 + c ₁)}}	
12 222I	4 2 _z	4 {{1, 0, 0}, {0, 1, 0}, {3 + 2c ₁ , 3 + 2c ₁ , 4(1 + c ₁)}}	
12 222I	4 2 _z	5 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c _{1}}}	
12 222I	5 222	1 {{1, 0, 0}, {0, 1, 0}, {3, 3, 4}}	
12 222I	5 222	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
12 222I	5 222	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
12 222I	5 222	4 {{1, 0, 0}, {0, 1, 0}, {3, 3, 4}}	

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
12 222I	5 222	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
12 222I	5 222	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
13 mm2P	2 2 _z	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
13 mm2P	2 2 _z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
13 mm2P	2 2 _z	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1 + c_1, 2 + 2c_1\}\}$	
13 mm2P	2 2 _z	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
13 mm2P	2 2 _z	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
13 mm2P	2 2 _z	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
13 mm2P	2 2 _z	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
13 mm2P	2 2 _z	8 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
13 mm2P	2 2 _z	9 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1 + c_1, 2 + 2c_1\}\}$	
13 mm2P	2 2 _z	10 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
13 mm2P	2 2 _z	11 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
13 mm2P	3 m _x	1 $\{\{1, 0, 0\}, \{1 + c_1, 2(1 + c_1), 0\}, \{1 + c_2, 0, 2(1 + c_2)\}\}$	
13 mm2P	3 m _x	2 $\{\{1, 0, 0\}, \{1 + c_1, 2(1 + c_1), 0\}, \{0, 0, 1 + c_2\}\}$	
13 mm2P	3 m _x	3 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 1 + c_2\}\}$	
13 mm2P	3 m _x	4 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 1 + c_2, 2(1 + c_2)\}\}$	
13 mm2P	3 m _x	5 $\{\{2, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 1 + c_2\}\}$	
13 mm2P	3 m _x	6 $\{\{2, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 1 + c_2, 2(1 + c_2)\}\}$	
13 mm2P	3 m _x	7 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1 + c_2, 0, 2(1 + c_2)\}\}$	
13 mm2P	3 m _x	8 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{2(1 + c_2), 2(1 + c_2), 4(1 + c_2)\}\}$	
13 mm2P	3 m _x	9 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{3 + 2c_2, 3 + 2c_2, 6 + 4c_2\}\}$	
13 mm2P	3 m _x	10 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1 + 2c_2, 1 + 2c_2, 2 + 4c_2\}\}$	
13 mm2P	3 m _x	11 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{2(1 + c_2), 2(1 + c_2), 4(1 + c_2)\}\}$	
13 mm2P	4 m _y	1 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 1 + c_2, 2(1 + c_2)\}\}$	
13 mm2P	4 m _y	2 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{2(1 + c_2), 2(1 + c_2), 4(1 + c_2)\}\}$	
13 mm2P	4 m _y	3 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + 2c_2, 1 + 2c_2, 2 + 4c_2\}\}$	
13 mm2P	4 m _y	4 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2(1 + c_2)\}\}$	
13 mm2P	4 m _y	5 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{2(1 + c_2), 0, 4(1 + c_2)\}\}$	
13 mm2P	4 m _y	6 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + 2c_2\}\}$	
13 mm2P	4 m _y	7 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + 2c_2, 0, 2 + 4c_2\}\}$	
13 mm2P	4 m _y	8 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_2\}\}$	
13 mm2P	4 m _y	9 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{1 + c_2, 0, 2(1 + c_2)\}\}$	
13 mm2P	4 m _y	10 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_2\}\}$	
13 mm2P	4 m _y	11 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{1 + c_2, 0, 2(1 + c_2)\}\}$	
13 mm2P	5 mm2 _z	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
13 mm2P	5 mm2 _z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
13 mm2P	5 mm2 _z	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1 + c_1, 2 + 2c_1\}\}$	
13 mm2P	5 mm2 _z	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
13 mm2P	5 mm2 _z	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
13 mm2P	5 mm2 _z	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
13 mm2P	5 mm2 _z	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
13 mm2P	5 mm2 _z	8 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
13 mm2P	5 mm2 _z	9 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1 + c_1, 2 + 2c_1\}\}$	
13 mm2P	5 mm2 _z	10 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
13 mm2P	5 mm2 _z	11 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
14 mm2C	2 2 _z	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
14 mm2C	2 2 _z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
14 mm2C	2 2 _z	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
14 mm2C	2 2 _z	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
14 mm2C	2 2 _z	5 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
14 mm2C	3 m _x	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1 + c_2\}\}$	
14 mm2C	3 m _x	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1 + c_2, 1 + c_2, 2(1 + c_2)\}\}$	
14 mm2C	4 m _y	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
14 mm2C	4 m _y	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2(1 + c_1)\}\}$	
14 mm2C	4 m _y	3 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 0, 1 + c_2\}\}$	
14 mm2C	4 m _y	4 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 1 + c_2, 2(1 + c_2)\}\}$	
14 mm2C	5 mm2 _z	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
14 mm2C	5 mm2 _z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
15 mm2A	2 2 _z	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + 2c_1, 2 + 2c_1\}\}$	
15 mm2A	2 2 _z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, c_1, 1 + c_1\}\}$	
15 mm2A	2 2 _z	3 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, c_1, 1 + c_1\}\}$	
15 mm2A	3 m _x	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
15 mm2A	3 m _x	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{3 + 2c_1, 2(1 + c_1), 2(2 + c_1)\}\}$	
15 mm2A	3 m _x	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{5 + 2c_1, 2, 4(2 + c_1)\}\}$	
15 mm2A	3 m _x	4 $\{\{1, 0, 0\}, \{2 + c_1, 2(2 + c_1), 0\}, \{2 + c_1, 0, 2(2 + c_1)\}\}$	
15 mm2A	3 m _x	5 $\{\{1, 0, 0\}, \{2 + c_1, 2(2 + c_1), 0\}, \{(2 + c_1)(3 + 2c_2), 2(2 + c_1)(3 + 2c_2)\}\}$	
15 mm2A	3 m _x	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{7 + 2d_1 + 2d_2, 2(2 + d_2), 2(5 + 2d_1 + d_2)\}\}$	27
15 mm2A	3 m _x	7 $\{\{1, 0, 0\}, \{2 + c_1, 2(2 + c_1), 0\}, \{(2 + c_1)(5 + 2d_1 + 2d_2), 2(2 + c_1)(1 + d_2), 2(2 + c_1)(4 + 2d_1 + d_2)\}\}$	26
15 mm2A	3 m _x	8 $\{\{1, 0, 0\}, \{2, 4, 0\}, \{2, 4, 8\}\}$	
15 mm2A	3 m _x	9 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 2, 2(2 + c_1)\}\}$	
15 mm2A	3 m _x	10 $\{\{1, 0, 0\}, \{3 + c_1, 2(3 + c_1), 0\}, \{3 + c_1, 2(3 + c_1), 4(3 + c_1)\}\}$	
15 mm2A	3 m _x	11 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{3 + 2d_1, 6 + 4d_1, 2(4 + 2d_1 + d_2)\}\}$	26
15 mm2A	3 m _x	12 $\{\{1, 0, 0\}, \{2, 4, 0\}, \{2 + 4d_1, 4 + 8d_1, 4(3 + 2d_1 + d_2)\}\}$	24
15 mm2A	3 m _x	13 $\{\{1, 0, 0\}, \{2, 4, 0\}, \{6 + 4d_1, 12 + 8d_1, 4(4 + 2d_1 + d_2)\}\}$	26

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
15 $mm2A$	3 m_x	14 $\{\{1, 0, 0\}, \{3 + c_1, 2(3 + c_1), 0\}, \{(3 + c_1)(1 + 2d_1), (3 + c_1)(2 + 4d_1), 2(3 + c_1)(3 + 2d_1 + d_2)\}\}$	24
15 $mm2A$	3 m_x	15 $\{\{1, 0, 0\}, \{3 + c_1, 2(3 + c_1), 0\}, \{(3 + c_1)(3 + 2d_1), 2(3 + c_1)(3 + 2d_1), 2(3 + c_1)(4 + 2d_1 + d_2)\}\}$	26
15 $mm2A$	3 m_x	16 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
15 $mm2A$	3 m_x	17 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 2, 6\}\}$	
15 $mm2A$	3 m_x	18 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 3 + c_1\}\}$	
15 $mm2A$	3 m_x	19 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1 + c_1, 2 + c_1\}\}$	
15 $mm2A$	3 m_x	20 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{0, 0, 2 + c_1\}\}$	
15 $mm2A$	3 m_x	21 $\{\{1, 0, 0\}, \{0, 3 + c_1, 0\}, \{0, 3 + c_1, 3(3 + c_1)\}\}$	
15 $mm2A$	3 m_x	22 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{0, (2 + c_1)(1 + c_2), (2 + c_1)(2 + c_2)\}\}$	
15 $mm2A$	3 m_x	23 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 2 + d_1, 4 + d_1 + d_2\}\}$	18
15 $mm2A$	3 m_x	24 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 2(1 + d_1), 2(4 + d_1 + d_2)\}\}$	16
15 $mm2A$	3 m_x	25 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 2(2 + d_1), 2(4 + d_1 + d_2)\}\}$	18
15 $mm2A$	3 m_x	26 $\{\{1, 0, 0\}, \{0, 3 + c_1, 0\}, \{0, (3 + c_1)(1 + d_1), (3 + c_1)(4 + d_1 + d_2)\}\}$	16
15 $mm2A$	3 m_x	27 $\{\{1, 0, 0\}, \{0, 3 + c_1, 0\}, \{0, (3 + c_1)(2 + d_1), (3 + c_1)(4 + d_1 + d_2)\}\}$	18
15 $mm2A$	3 m_x	28 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
15 $mm2A$	3 m_x	29 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 2, 6\}\}$	
15 $mm2A$	3 m_x	30 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 3 + c_1\}\}$	
15 $mm2A$	3 m_x	31 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1 + c_1, 2 + c_1\}\}$	
15 $mm2A$	3 m_x	32 $\{\{2, 0, 0\}, \{0, 2 + c_1, 0\}, \{0, 0, 2 + c_1\}\}$	
15 $mm2A$	3 m_x	33 $\{\{2, 0, 0\}, \{0, 3 + c_1, 0\}, \{0, 3 + c_1, 3(3 + c_1)\}\}$	
15 $mm2A$	3 m_x	34 $\{\{2, 0, 0\}, \{0, 2 + c_1, 0\}, \{0, (2 + c_1)(1 + c_2), (2 + c_1)(2 + c_2)\}\}$	
15 $mm2A$	3 m_x	35 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 2 + d_1, 4 + d_1 + d_2\}\}$	18
15 $mm2A$	3 m_x	36 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 2(1 + d_1), 2(4 + d_1 + d_2)\}\}$	16
15 $mm2A$	3 m_x	37 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 2(2 + d_1), 2(4 + d_1 + d_2)\}\}$	18
15 $mm2A$	3 m_x	38 $\{\{2, 0, 0\}, \{0, 3 + c_1, 0\}, \{0, (3 + c_1)(1 + d_1), (3 + c_1)(4 + d_1 + d_2)\}\}$	16
15 $mm2A$	3 m_x	39 $\{\{2, 0, 0\}, \{0, 3 + c_1, 0\}, \{0, (3 + c_1)(2 + d_1), (3 + c_1)(4 + d_1 + d_2)\}\}$	18
15 $mm2A$	3 m_x	40 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{2, 2, 4\}\}$	
15 $mm2A$	3 m_x	41 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{4, 2, 8\}\}$	
15 $mm2A$	3 m_x	42 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{4(1 + c_1), 6(1 + c_1), 8(1 + c_1)\}\}$	
15 $mm2A$	3 m_x	43 $\{\{1, 0, 0\}, \{0, 2(2 + c_1), 0\}, \{2(2 + c_1), 2(2 + c_1), 4(2 + c_1)\}\}$	
15 $mm2A$	3 m_x	44 $\{\{1, 0, 0\}, \{0, 2(2 + c_1), 0\}, \{4(2 + c_1), 2(2 + c_1), 8(2 + c_1)\}\}$	
15 $mm2A$	3 m_x	45 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{2(1 + c_1)(3 + c_2), 2(1 + c_1)(5 + 2c_2), 4(1 + c_1)(3 + c_2)\}\}$	
15 $mm2A$	3 m_x	46 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{2(4 + d_1 + 2d_2), 6 + 4d_1 + 4d_2, 4(4 + d_1 + 2d_2)\}\}$	39
15 $mm2A$	3 m_x	47 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{2(4 + d_1 + 2d_2), 10 + 4d_1 + 4d_2, 4(4 + d_1 + 2d_2)\}\}$	40
15 $mm2A$	3 m_x	48 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{2(3 + d_1 + 2d_2), 2 + 4d_1 + 4d_2, 4(3 + d_1 + 2d_2)\}\}$	42
15 $mm2A$	3 m_x	49 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{2(3 + d_1 + 2d_2), 6 + 4d_1 + 4d_2, 4(3 + d_1 + 2d_2)\}\}$	41
15 $mm2A$	3 m_x	50 $\{\{1, 0, 0\}, \{0, 2(2 + c_1), 0\}, \{2(2 + c_1)(3 + d_1 + d_2), 2(2 + c_1)(1 + 2d_1), 4(2 + c_1)(3 + d_1 + d_2)\}\}$	9
15 $mm2A$	3 m_x	51 $\{\{1, 0, 0\}, \{0, 2(2 + c_1), 0\}, \{2(2 + c_1)(3 + d_1 + d_2), 2(2 + c_1)(3 + 2d_1), 4(2 + c_1)(3 + d_1 + d_2)\}\}$	12
15 $mm2A$	3 m_x	52 $\{\{1, 0, 0\}, \{0, 2(2 + c_1), 0\}, \{4(2 + c_1), 6(2 + c_1), 8(2 + c_1)\}\}$	
15 $mm2A$	3 m_x	53 $\{\{1, 0, 0\}, \{0, 1 + 2c_1, 0\}, \{2 + 4c_1, 1 + 2c_1, 4 + 8c_1\}\}$	
15 $mm2A$	3 m_x	54 $\{\{1, 0, 0\}, \{0, 3 + 2c_1, 0\}, \{3 + 2c_1, 3 + 2c_1, 6 + 4c_1\}\}$	
15 $mm2A$	3 m_x	55 $\{\{1, 0, 0\}, \{0, 3 + 2c_1, 0\}, \{9 + 6c_1, 5(3 + 2c_1), 6(3 + 2c_1)\}\}$	
15 $mm2A$	3 m_x	56 $\{\{1, 0, 0\}, \{0, 1 + 2c_1, 0\}, \{(1 + 2c_1)(3 + c_2), 1 + 2c_1, 2(1 + 2c_1)(3 + c_2)\}\}$	
15 $mm2A$	3 m_x	57 $\{\{1, 0, 0\}, \{0, 3 + 2c_1, 0\}, \{(3 + 2c_1)(4 + c_2), (3 + 2c_1)(7 + 2c_2), 2(3 + 2c_1)(4 + c_2)\}\}$	
15 $mm2A$	3 m_x	58 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{4 + d_1 + d_2, 3 + 2d_1, 2(4 + d_1 + d_2)\}\}$	17
15 $mm2A$	3 m_x	59 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{4 + d_1 + d_2, 5 + 2d_1, 2(4 + d_1 + d_2)\}\}$	19
15 $mm2A$	3 m_x	60 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{2(1 + c_1)(4 + d_1 + d_2), 2(1 + c_1)(3 + 2d_1), 4(1 + c_1)(4 + d_1 + d_2)\}\}$	17
15 $mm2A$	3 m_x	61 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{2(1 + c_1)(4 + d_1 + d_2), 2(1 + c_1)(5 + 2d_1), 4(1 + c_1)(4 + d_1 + d_2)\}\}$	19
15 $mm2A$	3 m_x	62 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{2, 3, 4\}\}$	
15 $mm2A$	3 m_x	63 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{4(1 + c_1), 6(1 + c_1), 8(1 + c_1)\}\}$	
15 $mm2A$	3 m_x	64 $\{\{1, 0, 0\}, \{0, 1 + 2c_1, 0\}, \{1 + 2c_1, 1 + 2c_1, 2 + 4c_1\}\}$	
15 $mm2A$	3 m_x	65 $\{\{1, 0, 0\}, \{0, 1 + 2c_1, 0\}, \{(1 + 2c_1)(2 + c_2), 1 + 2c_1, 2(1 + 2c_1)(2 + c_2)\}\}$	
15 $mm2A$	3 m_x	66 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + d_1 + d_2, 3 + 2d_1, 2(3 + d_1 + d_2)\}\}$	12
15 $mm2A$	3 m_x	67 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + d_1 + d_2, 5 + 2d_1, 2(3 + d_1 + d_2)\}\}$	15
15 $mm2A$	3 m_x	68 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{2(1 + c_1)(3 + d_1 + d_2), 2(1 + c_1)(3 + 2d_1), 4(1 + c_1)(3 + d_1 + d_2)\}\}$	12
15 $mm2A$	3 m_x	69 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{2(1 + c_1)(3 + d_1 + d_2), 2(1 + c_1)(5 + 2d_1), 4(1 + c_1)(3 + d_1 + d_2)\}\}$	15
15 $mm2A$	3 m_x	70 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{4, 6, 8\}\}$	
15 $mm2A$	3 m_x	71 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{2(1 + c_1), 2(1 + c_1), 4(1 + c_1)\}\}$	
15 $mm2A$	3 m_x	72 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{6(1 + c_1), 10(1 + c_1), 12(1 + c_1)\}\}$	
15 $mm2A$	3 m_x	73 $\{\{1, 0, 0\}, \{0, 2(2 + c_1), 0\}, \{4(2 + c_1), 6(2 + c_1), 8(2 + c_1)\}\}$	
15 $mm2A$	3 m_x	74 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{2(1 + c_1)(2 + c_2), 2(1 + c_1), 4(1 + c_1)(2 + c_2)\}\}$	
15 $mm2A$	3 m_x	75 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{2(1 + c_1)(4 + c_2), 2(1 + c_1)(7 + 2c_2), 4(1 + c_1)(4 + c_2)\}\}$	
15 $mm2A$	3 m_x	76 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{2(1 + c_1)(4 + d_1 + d_2), 2(1 + c_1)(3 + 2d_1), 4(1 + c_1)(4 + d_1 + d_2)\}\}$	17
15 $mm2A$	3 m_x	77 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{2(1 + c_1)(4 + d_1 + d_2), 2(1 + c_1)(5 + 2d_1), 4(1 + c_1)(4 + d_1 + d_2)\}\}$	19
15 $mm2A$	4 m_y	1 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, c_2, 1 + c_2\}\}$	
15 $mm2A$	4 m_y	2 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + c_2, 1 + 2c_2, 2(1 + c_2)\}\}$	
15 $mm2A$	5 $mm2_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + 2c_1, 2 + 2c_1\}\}$	
15 $mm2A$	5 $mm2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, c_1, 1 + c_1\}\}$	
15 $mm2A$	5 $mm2_z$	3 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, c_1, 1 + c_1\}\}$	
16 $mm2F$	2 2_z	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 0, 2\}\}$	
16 $mm2F$	2 2_z	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 1, 2\}\}$	
16 $mm2F$	2 2_z	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
16 $mm2F$	3 m_x	1 $\{\{1, 0, 0\}, \{c_2, 1 + c_2, 0\}, \{c_1, 0, 1 + c_1\}\}$	
16 $mm2F$	3 m_x	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{c_2, 1 + c_2, 2(1 + c_2)\}\}$	
16 $mm2F$	4 m_y	1 $\{\{1, 0, 0\}, \{(1 + c_1)c_2, 1 + c_2 + c_1c_2, 0\}, \{0, c_1, 1 + c_1\}\}$	
16 $mm2F$	4 m_y	2 $\{\{1, 0, 0\}, \{(1 + c_1)(1 + 2c_2), 2 + c_1 + 2c_2 + 2c_1c_2, 0\}, \{0, 1 + 2c_1, 2(1 + c_1)\}\}$	
16 $mm2F$	4 m_y	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 0, 2(1 + c_1)\}\}$	

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
16 $mm2F$	4 m_y	4 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{2(1 + c_2), 1 + 2c_2, 2(2 + c_1 + 2c_2)\}\}$	
16 $mm2F$	4 m_y	5 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{3 + 2c_2, 2(1 + c_2), 2(3 + c_1 + 2c_2)\}\}$	
16 $mm2F$	4 m_y	6 $\{\{1, 0, 0\}, \{1 + 2c_3 + 2c_1(1 + c_2 + c_3), 2(1 + c_3 + c_1(1 + c_2 + c_3)), 0\}, \{1 + 2c_2, 2c_2, 2(1 + c_2 + c_3)\}\}$	
16 $mm2F$	4 m_y	7 $\{\{1, 0, 0\}, \{2 + c_2 + 3c_3 + 2c_1(1 + c_2 + c_3), 3 + c_2 + 3c_3 + 2c_1(1 + c_2 + c_3), 0\}, \{1 + 2c_2, 2c_2, 2(1 + c_2 + c_3)\}\}$	
16 $mm2F$	4 m_y	8 $\{\{1, 0, 0\}, \{2(1 + c_3 + c_1(2 + c_2 + c_3)), 3 + 2c_3 + 2c_1(2 + c_2 + c_3), 0\}, \{2(1 + c_2), 1 + 2c_2, 2(2 + c_2 + c_3)\}\}$	
16 $mm2F$	4 m_y	9 $\{\{1, 0, 0\}, \{4 + c_2 + 3c_3 + 2c_1(2 + c_2 + c_3), 5 + c_2 + 3c_3 + 2c_1(2 + c_2 + c_3), 0\}, \{2(1 + c_2), 1 + 2c_2, 2(2 + c_2 + c_3)\}\}$	
16 $mm2F$	4 m_y	10 $\{\{1, 0, 0\}, \{1 + 2c_3 + c_1(3 + 2c_2 + 2c_3), 2(1 + c_3) + c_1(3 + 2c_2 + 2c_3), 0\}, \{2(1 + c_2), 1 + 2c_2, 3 + 2c_2 + 2c_3\}\}$	
16 $mm2F$	4 m_y	11 $\{\{1, 0, 0\}, \{2(1 + c_3) + c_1(3 + 2c_2 + 2c_3), 3 + 2c_3 + c_1(3 + 2c_2 + 2c_3), 0\}, \{1 + 2c_2, 2c_2, 3 + 2c_2 + 2c_3\}\}$	
16 $mm2F$	5 $mm2_z$	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 0, 2\}\}$	
16 $mm2F$	5 $mm2_z$	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 1, 2\}\}$	
16 $mm2F$	5 $mm2_z$	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
17 $mm2I$	2 2_z	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
17 $mm2I$	2 2_z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
17 $mm2I$	2 2_z	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{2, 2, 2(2 + c_1)\}\}$	
17 $mm2I$	2 2_z	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + 2c_1, 3 + 2c_1, 4(1 + c_1)\}\}$	
17 $mm2I$	2 2_z	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2 + c_1\}\}$	
17 $mm2I$	3 m_x	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
17 $mm2I$	3 m_x	2 $\{\{2 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2 + c_1\}\}$	
17 $mm2I$	3 m_x	3 $\{\{2 + c_1, 0, 0\}, \{0, 1, 0\}, \{(2 + c_1)(1 + c_2), 1, (2 + c_1)(2 + c_2)\}\}$	
17 $mm2I$	3 m_x	4 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{(1 + c_1)(1 + d_1), 1, (1 + c_1)(3 + d_1 + d_2)\}\}$	10
17 $mm2I$	3 m_x	5 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1, 2(1 + c_1)\}\}$	
17 $mm2I$	3 m_x	6 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1, (1 + c_1)(3 + c_2)\}\}$	
17 $mm2I$	3 m_x	7 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{(1 + c_1)(2 + d_1), 1, (1 + c_1)(3 + d_1 + d_2)\}\}$	13
17 $mm2I$	4 m_y	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
17 $mm2I$	4 m_y	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 3\}\}$	
17 $mm2I$	4 m_y	3 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 2, 8\}\}$	
17 $mm2I$	4 m_y	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 4 + c_1\}\}$	
17 $mm2I$	4 m_y	5 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, 0, 2 + c_1\}\}$	
17 $mm2I$	4 m_y	6 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, 2 + c_1, 3(2 + c_1)\}\}$	
17 $mm2I$	4 m_y	7 $\{\{1, 0, 0\}, \{0, 3 + c_1, 0\}, \{1, 3 + c_1, 4(3 + c_1)\}\}$	
17 $mm2I$	4 m_y	8 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, (2 + c_1)(1 + c_2), (2 + c_1)(2 + c_2)\}\}$	
17 $mm2I$	4 m_y	9 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 2 + d_1, 5 + d_1 + d_2\}\}$	21
17 $mm2I$	4 m_y	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 2(1 + d_1), 2(5 + d_1 + d_2)\}\}$	20
17 $mm2I$	4 m_y	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 2(2 + d_1), 2(5 + d_1 + d_2)\}\}$	21
17 $mm2I$	4 m_y	12 $\{\{1, 0, 0\}, \{0, 3 + c_1, 0\}, \{1, (3 + c_1)(1 + d_1), (3 + c_1)(5 + d_1 + d_2)\}\}$	20
17 $mm2I$	4 m_y	13 $\{\{1, 0, 0\}, \{0, 3 + c_1, 0\}, \{1, (3 + c_1)(2 + d_1), (3 + c_1)(5 + d_1 + d_2)\}\}$	21
17 $mm2I$	4 m_y	14 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 2 + c_1, 3 + c_1\}\}$	
17 $mm2I$	4 m_y	15 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1, 1 + c_1, 2(1 + c_1)\}\}$	
17 $mm2I$	4 m_y	16 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1, 1 + c_1, (1 + c_1)(3 + c_2)\}\}$	
17 $mm2I$	4 m_y	17 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, (2 + c_1)(2 + c_2), (2 + c_1)(3 + c_2)\}\}$	
17 $mm2I$	4 m_y	18 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 3 + d_1, 5 + d_1 + d_2\}\}$	22
17 $mm2I$	4 m_y	19 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, (2 + c_1)(2 + d_1), (2 + c_1)(5 + d_1 + d_2)\}\}$	21
17 $mm2I$	4 m_y	20 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, (2 + c_1)(3 + d_1), (2 + c_1)(5 + d_1 + d_2)\}\}$	22
17 $mm2I$	5 $mm2_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
17 $mm2I$	5 $mm2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2 + c_1\}\}$	
18 $mmmP$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
18 $mmmP$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
18 $mmmP$	2 $\bar{1}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
18 $mmmP$	2 $\bar{1}$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
18 $mmmP$	2 $\bar{1}$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 $mmmP$	2 $\bar{1}$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
18 $mmmP$	2 $\bar{1}$	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
18 $mmmP$	2 $\bar{1}$	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
18 $mmmP$	2 $\bar{1}$	9 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
18 $mmmP$	2 $\bar{1}$	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
18 $mmmP$	2 $\bar{1}$	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
18 $mmmP$	2 $\bar{1}$	12 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
18 $mmmP$	2 $\bar{1}$	13 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
18 $mmmP$	2 $\bar{1}$	14 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 $mmmP$	2 $\bar{1}$	15 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
18 $mmmP$	2 $\bar{1}$	16 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
18 $mmmP$	3 2_x	1 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
18 $mmmP$	3 2_x	2 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
18 $mmmP$	3 2_x	3 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
18 $mmmP$	3 2_x	4 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 $mmmP$	3 2_x	5 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
18 $mmmP$	3 2_x	6 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
18 $mmmP$	3 2_x	7 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
18 $mmmP$	3 2_x	8 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
18 $mmmP$	3 2_x	9 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
18 $mmmP$	3 2_x	10 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	

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Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
18 mmmP	3 2_x	11 $\{\{1+c_1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
18 mmmP	4 2_y	1 $\{\{1, 0, 0\}, \{1+c_1, 2+2c_1, 0\}, \{0, 0, 1\}\}$	
18 mmmP	4 2_y	2 $\{\{1, 0, 0\}, \{0, 1+c_1, 0\}, \{0, 0, 1\}\}$	
18 mmmP	4 2_y	3 $\{\{1, 0, 0\}, \{1+c_1, 2+2c_1, 0\}, \{1, 0, 2\}\}$	
18 mmmP	4 2_y	4 $\{\{1, 0, 0\}, \{1+c_1, 2+2c_1, 0\}, \{0, 0, 2\}\}$	
18 mmmP	4 2_y	5 $\{\{1, 0, 0\}, \{0, 1+c_1, 0\}, \{1, 0, 2\}\}$	
18 mmmP	4 2_y	6 $\{\{1, 0, 0\}, \{0, 1+c_1, 0\}, \{1, 1, 2\}\}$	
18 mmmP	4 2_y	7 $\{\{1, 0, 0\}, \{0, 1+c_1, 0\}, \{0, 0, 2\}\}$	
18 mmmP	4 2_y	8 $\{\{1, 0, 0\}, \{0, 1+c_1, 0\}, \{0, 1, 2\}\}$	
18 mmmP	4 2_y	9 $\{\{2, 0, 0\}, \{0, 1+c_1, 0\}, \{0, 0, 1\}\}$	
18 mmmP	4 2_y	10 $\{\{2, 0, 0\}, \{0, 1+c_1, 0\}, \{0, 0, 2\}\}$	
18 mmmP	4 2_y	11 $\{\{2, 0, 0\}, \{0, 1+c_1, 0\}, \{0, 1, 2\}\}$	
18 mmmP	5 2_z	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
18 mmmP	5 2_z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1+c_1, 0, 2+2c_1\}\}$	
18 mmmP	5 2_z	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1+c_1, 2+2c_1\}\}$	
18 mmmP	5 2_z	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1+c_1\}\}$	
18 mmmP	5 2_z	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1+c_1, 0, 2+2c_1\}\}$	
18 mmmP	5 2_z	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1+c_1\}\}$	
18 mmmP	5 2_z	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1+c_1, 0, 2+2c_1\}\}$	
18 mmmP	5 2_z	8 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1+c_1\}\}$	
18 mmmP	5 2_z	9 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1+c_1, 2+2c_1\}\}$	
18 mmmP	5 2_z	10 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1+c_1\}\}$	
18 mmmP	5 2_z	11 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1+c_1\}\}$	
18 mmmP	6 m_x	1 $\{\{1, 0, 0\}, \{1+c_1, 2(1+c_1), 0\}, \{1+c_2, 0, 2(1+c_2)\}\}$	
18 mmmP	6 m_x	2 $\{\{1, 0, 0\}, \{1+c_1, 2(1+c_1), 0\}, \{0, 0, 1+c_2\}\}$	
18 mmmP	6 m_x	3 $\{\{1, 0, 0\}, \{0, 1+c_1, 0\}, \{0, 0, 1+c_2\}\}$	
18 mmmP	6 m_x	4 $\{\{1, 0, 0\}, \{0, 1+c_1, 0\}, \{0, 1+c_2, 2(1+c_2)\}\}$	
18 mmmP	6 m_x	5 $\{\{2, 0, 0\}, \{0, 1+c_1, 0\}, \{0, 0, 1+c_2\}\}$	
18 mmmP	6 m_x	6 $\{\{2, 0, 0\}, \{0, 1+c_1, 0\}, \{0, 1+c_2, 2(1+c_2)\}\}$	
18 mmmP	6 m_x	7 $\{\{1, 0, 0\}, \{0, 1+c_1, 0\}, \{1+c_2, 0, 2(1+c_2)\}\}$	
18 mmmP	6 m_x	8 $\{\{1, 0, 0\}, \{0, 1+c_1, 0\}, \{2(1+c_2), 2(1+c_2), 4(1+c_2)\}\}$	
18 mmmP	6 m_x	9 $\{\{1, 0, 0\}, \{0, 1+c_1, 0\}, \{3+2c_2, 3+2c_2, 6+4c_2\}\}$	
18 mmmP	6 m_x	10 $\{\{1, 0, 0\}, \{0, 1+c_1, 0\}, \{1+2c_2, 1+2c_2, 2+4c_2\}\}$	
18 mmmP	6 m_x	11 $\{\{1, 0, 0\}, \{0, 1+c_1, 0\}, \{2(1+c_2), 2(1+c_2), 4(1+c_2)\}\}$	
18 mmmP	7 m_y	1 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{0, 1+c_2, 2(1+c_2)\}\}$	
18 mmmP	7 m_y	2 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{2(1+c_2), 2(1+c_2), 4(1+c_2)\}\}$	
18 mmmP	7 m_y	3 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{1+2c_2, 1+2c_2, 2+4c_2\}\}$	
18 mmmP	7 m_y	4 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2(1+c_2)\}\}$	
18 mmmP	7 m_y	5 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{2(1+c_2), 0, 4(1+c_2)\}\}$	
18 mmmP	7 m_y	6 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1+2c_2\}\}$	
18 mmmP	7 m_y	7 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{1+2c_2, 0, 2+4c_2\}\}$	
18 mmmP	7 m_y	8 $\{\{1+c_1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1+c_2\}\}$	
18 mmmP	7 m_y	9 $\{\{1+c_1, 0, 0\}, \{0, 2, 0\}, \{1+c_2, 0, 2(1+c_2)\}\}$	
18 mmmP	7 m_y	10 $\{\{1+c_1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1+c_2\}\}$	
18 mmmP	7 m_y	11 $\{\{1+c_1, 0, 0\}, \{1, 2, 0\}, \{1+c_2, 0, 2(1+c_2)\}\}$	
18 mmmP	8 m_z	1 $\{\{1+c_1, 0, 0\}, \{0, 1+c_2, 0\}, \{0, 0, 1\}\}$	
18 mmmP	8 m_z	2 $\{\{1+c_1, 0, 0\}, \{1+c_2, 2(1+c_2), 0\}, \{0, 0, 1\}\}$	
18 mmmP	8 m_z	3 $\{\{1+c_1, 0, 0\}, \{0, 1+c_2, 0\}, \{0, 0, 2\}\}$	
18 mmmP	8 m_z	4 $\{\{1+c_1, 0, 0\}, \{1+c_2, 2(1+c_2), 0\}, \{0, 0, 2\}\}$	
18 mmmP	8 m_z	5 $\{\{1+c_1, 0, 0\}, \{0, 1+c_2, 0\}, \{0, 1, 2\}\}$	
18 mmmP	8 m_z	6 $\{\{1+c_1, 0, 0\}, \{0, 1+c_2, 0\}, \{1, 0, 2\}\}$	
18 mmmP	8 m_z	7 $\{\{1+c_1, 0, 0\}, \{1+c_2, 2(1+c_2), 0\}, \{1, 0, 2\}\}$	
18 mmmP	8 m_z	8 $\{\{1+c_1, 0, 0\}, \{0, 1+c_2, 0\}, \{1, 1, 2\}\}$	
18 mmmP	9 $2/m_x$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
18 mmmP	9 $2/m_x$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
18 mmmP	9 $2/m_x$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
18 mmmP	9 $2/m_x$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
18 mmmP	9 $2/m_x$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 mmmP	9 $2/m_x$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
18 mmmP	9 $2/m_x$	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
18 mmmP	9 $2/m_x$	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
18 mmmP	9 $2/m_x$	9 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
18 mmmP	9 $2/m_x$	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
18 mmmP	9 $2/m_x$	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
18 mmmP	9 $2/m_x$	12 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
18 mmmP	9 $2/m_x$	13 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
18 mmmP	9 $2/m_x$	14 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 mmmP	9 $2/m_x$	15 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
18 mmmP	9 $2/m_x$	16 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
18 mmmP	10 $2/m_y$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
18 mmmP	10 $2/m_y$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
18 mmmP	10 $2/m_y$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
18 mmmP	10 $2/m_y$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
18 mmmP	10 $2/m_y$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 mmmP	10 $2/m_y$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
18 mmmP	10 $2/m_y$	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
18 mmmP	10 $2/m_y$	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
18	$mmmP$	10 $\{2/m_y\}$	9 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	10 $\{2/m_y\}$	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	10 $\{2/m_y\}$	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	10 $\{2/m_y\}$	12 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	10 $\{2/m_y\}$	13 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$
18	$mmmP$	10 $\{2/m_y\}$	14 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	10 $\{2/m_y\}$	15 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	10 $\{2/m_y\}$	16 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	11 $\{2/m_z\}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	11 $\{2/m_z\}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$
18	$mmmP$	11 $\{2/m_z\}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	11 $\{2/m_z\}$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$
18	$mmmP$	11 $\{2/m_z\}$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	11 $\{2/m_z\}$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	11 $\{2/m_z\}$	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	11 $\{2/m_z\}$	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	11 $\{2/m_z\}$	9 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	11 $\{2/m_z\}$	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	11 $\{2/m_z\}$	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	11 $\{2/m_z\}$	12 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	11 $\{2/m_z\}$	13 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$
18	$mmmP$	11 $\{2/m_z\}$	14 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	11 $\{2/m_z\}$	15 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	11 $\{2/m_z\}$	16 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	12 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	12 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$
18	$mmmP$	12 222	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	12 222	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$
18	$mmmP$	12 222	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	12 222	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	12 222	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	12 222	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	12 222	9 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	12 222	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	12 222	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	12 222	12 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	12 222	13 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$
18	$mmmP$	12 222	14 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	12 222	15 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	12 222	16 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	13 2_xmm	1 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	13 2_xmm	2 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$
18	$mmmP$	13 2_xmm	3 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$
18	$mmmP$	13 2_xmm	4 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	13 2_xmm	5 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	13 2_xmm	6 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	13 2_xmm	7 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	13 2_xmm	8 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	13 2_xmm	9 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	13 2_xmm	10 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	13 2_xmm	11 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	14 $m2_y m$	1 $\{\{1, 0, 0\}, \{1 + c_1, 2 + 2c_1, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	14 $m2_y m$	2 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	14 $m2_y m$	3 $\{\{1, 0, 0\}, \{1 + c_1, 2 + 2c_1, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	14 $m2_y m$	4 $\{\{1, 0, 0\}, \{1 + c_1, 2 + 2c_1, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	14 $m2_y m$	5 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	14 $m2_y m$	6 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1, 1, 2\}\}$
18	$mmmP$	14 $m2_y m$	7 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	14 $m2_y m$	8 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 1, 2\}\}$
18	$mmmP$	14 $m2_y m$	9 $\{\{2, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	14 $m2_y m$	10 $\{\{2, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 2\}\}$
18	$mmmP$	14 $m2_y m$	11 $\{\{2, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 1, 2\}\}$
18	$mmmP$	15 $mm2_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$
18	$mmmP$	15 $mm2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$
18	$mmmP$	15 $mm2_z$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1 + c_1, 2 + 2c_1\}\}$
18	$mmmP$	15 $mm2_z$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$
18	$mmmP$	15 $mm2_z$	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$
18	$mmmP$	15 $mm2_z$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$
18	$mmmP$	15 $mm2_z$	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$
18	$mmmP$	15 $mm2_z$	8 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$
18	$mmmP$	15 $mm2_z$	9 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1 + c_1, 2 + 2c_1\}\}$
18	$mmmP$	15 $mm2_z$	10 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$
18	$mmmP$	15 $mm2_z$	11 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$
18	$mmmP$	16 mmm	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$
18	$mmmP$	16 mmm	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$
18	$mmmP$	16 mmm	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$
18	$mmmP$	16 mmm	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$

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Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
18 $mmmP$	16 mmm	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 $mmmP$	16 mmm	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
18 $mmmP$	16 mmm	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
18 $mmmP$	16 mmm	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
18 $mmmP$	16 mmm	9 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
18 $mmmP$	16 mmm	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
18 $mmmP$	16 mmm	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
18 $mmmP$	16 mmm	12 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
18 $mmmP$	16 mmm	13 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
18 $mmmP$	16 mmm	14 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 $mmmP$	16 mmm	15 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
18 $mmmP$	16 mmm	16 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
19 $mmmC$	2 $\bar{1}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	2 $\bar{1}$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	2 $\bar{1}$	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
19 $mmmC$	2 $\bar{1}$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	2 $\bar{1}$	7 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	2 $\bar{1}$	8 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	3 2_x	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	3 2_x	2 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	3 2_x	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
19 $mmmC$	3 2_x	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	3 2_x	5 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	3 2_x	6 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 1, 2\}\}$	
19 $mmmC$	4 2_y	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	4 2_y	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	4 2_y	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 1, 2\}\}$	
19 $mmmC$	5 2_z	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
19 $mmmC$	5 2_z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
19 $mmmC$	5 2_z	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
19 $mmmC$	5 2_z	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
19 $mmmC$	5 2_z	5 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
19 $mmmC$	6 m_x	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1 + c_2\}\}$	
19 $mmmC$	6 m_x	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1 + c_2, 1 + c_2, 2(1 + c_2)\}\}$	
19 $mmmC$	7 m_y	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
19 $mmmC$	7 m_y	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2(1 + c_1)\}\}$	
19 $mmmC$	7 m_y	3 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 0, 1 + c_2\}\}$	
19 $mmmC$	7 m_y	4 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 1 + c_2, 2(1 + c_2)\}\}$	
19 $mmmC$	8 m_z	1 $\{\{1 + c_1, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	8 m_z	2 $\{\{1 + c_1, 0, 0\}, \{(1 + c_1)(1 + d_1), (1 + c_1)(2 + d_1 + d_2), 0\}, \{0, 0, 1\}\}$	5
19 $mmmC$	8 m_z	3 $\{\{1 + c_1, 0, 0\}, \{0, 1 + c_1, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	8 m_z	4 $\{\{1 + c_1, 0, 0\}, \{(1 + c_1)(1 + d_1), (1 + c_1)(2 + d_1 + d_2), 0\}, \{0, 0, 2\}\}$	5
19 $mmmC$	8 m_z	5 $\{\{1 + c_1, 0, 0\}, \{(1 + c_1)(1 + 2c_2), 2(1 + c_1)(1 + c_2), 0\}, \{0, 1, 2\}\}$	
19 $mmmC$	8 m_z	6 $\{\{1 + c_1, 0, 0\}, \{(1 + c_1)(1 + 2d_1), (1 + c_1)(3 + 2d_1 + d_2), 0\}, \{0, 1, 2\}\}$	24
19 $mmmC$	8 m_z	7 $\{\{1 + c_1, 0, 0\}, \{(1 + c_1)(1 + 2c_2), 2(1 + c_1)(1 + c_2), 0\}, \{1, 0, 2\}\}$	
19 $mmmC$	8 m_z	8 $\{\{1 + c_1, 0, 0\}, \{(1 + c_1)(1 + 2d_1), 2(1 + c_1)(2 + d_1 + d_2), 0\}, \{1, 0, 2\}\}$	4
19 $mmmC$	8 m_z	9 $\{\{1 + c_1, 0, 0\}, \{(1 + c_1)d_1, (1 + c_1)(1 + d_1 + 2d_2), 0\}, \{1, 1, 2\}\}$	38
19 $mmmC$	9 $2/m_x$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	9 $2/m_x$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	9 $2/m_x$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	9 $2/m_x$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
19 $mmmC$	9 $2/m_x$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	10 $2/m_y$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	10 $2/m_y$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	10 $2/m_y$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	10 $2/m_y$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
19 $mmmC$	10 $2/m_y$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	11 $2/m_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	11 $2/m_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
19 $mmmC$	11 $2/m_z$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	11 $2/m_z$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	11 $2/m_z$	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
19 $mmmC$	11 $2/m_z$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	11 $2/m_z$	7 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	11 $2/m_z$	8 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	12 222	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	12 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	12 222	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	12 222	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
19 $mmmC$	12 222	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	13 $2_x mm$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	13 $2_x mm$	2 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	13 $2_x mm$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
19 $mmmC$	13 $2_x mm$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	13 $2_x mm$	5 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 0, 2\}\}$	

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Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
19 $mmmC$	13 $2_x mm$	6 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 1, 2\}\}$	
19 $mmmC$	14 $m2_y m$	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	14 $m2_y m$	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	14 $m2_y m$	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 1, 2\}\}$	
19 $mmmC$	15 $mm2_z$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
19 $mmmC$	15 $mm2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
19 $mmmC$	15 $mm2_z$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
19 $mmmC$	16 mmm	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	16 mmm	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
19 $mmmC$	16 mmm	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
19 $mmmC$	16 mmm	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
19 $mmmC$	16 mmm	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
20 $mmmF$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
20 $mmmF$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
20 $mmmF$	2 $\bar{1}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
20 $mmmF$	2 $\bar{1}$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
20 $mmmF$	2 $\bar{1}$	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
20 $mmmF$	2 $\bar{1}$	6 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
20 $mmmF$	3 2_x	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
20 $mmmF$	3 2_x	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, c_1, 2 + c_1\}\}$	
20 $mmmF$	3 2_x	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, c_1, 1 + c_1\}\}$	
20 $mmmF$	3 2_x	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, c_1, 2 + 2c_1\}\}$	
20 $mmmF$	4 2_y	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{c_1, 0, 1 + c_1\}\}$	
20 $mmmF$	4 2_y	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{c_1, 1 + c_1, 2 + 2c_1\}\}$	
20 $mmmF$	4 2_y	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{c_1, 0, 1 + c_1\}\}$	
20 $mmmF$	5 2_z	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 0, 2\}\}$	
20 $mmmF$	5 2_z	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 1, 2\}\}$	
20 $mmmF$	5 2_z	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
20 $mmmF$	6 m_x	1 $\{\{1, 0, 0\}, \{c_2, 1 + c_2, 0\}, \{c_1, 0, 1 + c_1\}\}$	
20 $mmmF$	6 m_x	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{c_2, 1 + c_2, 2(1 + c_2)\}\}$	
20 $mmmF$	7 m_y	1 $\{\{1, 0, 0\}, \{(1 + c_1)c_2, 1 + c_2 + c_1c_2, 0\}, \{0, c_1, 1 + c_1\}\}$	
20 $mmmF$	7 m_y	2 $\{\{1, 0, 0\}, \{(1 + c_1)(1 + 2c_2), 2 + c_1 + 2c_2 + 2c_1c_2, 0\}, \{0, 1 + 2c_1, 2(1 + c_1)\}\}$	
20 $mmmF$	7 m_y	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 0, 2(1 + c_1)\}\}$	
20 $mmmF$	7 m_y	4 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{2(1 + c_2), 1 + 2c_2, 2(2 + c_1 + 2c_2)\}\}$	
20 $mmmF$	7 m_y	5 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{3 + 2c_2, 2(1 + c_2), 2(3 + c_1 + 2c_2)\}\}$	
20 $mmmF$	7 m_y	6 $\{\{1, 0, 0\}, \{1 + 2c_3 + 2c_1(1 + c_2 + c_3), 2(1 + c_3 + c_1(1 + c_2 + c_3)), 0\}, \{1 + 2c_2, 2c_2, 2(1 + c_2 + c_3)\}\}$	
20 $mmmF$	7 m_y	7 $\{\{1, 0, 0\}, \{2 + c_2 + 3c_3 + 2c_1(1 + c_2 + c_3), 3 + c_2 + 3c_3 + 2c_1(1 + c_2 + c_3), 0\}, \{1 + 2c_2, 2c_2, 2(1 + c_2 + c_3)\}\}$	
20 $mmmF$	7 m_y	8 $\{\{1, 0, 0\}, \{2(1 + c_3 + c_1(2 + c_2 + c_3)), 3 + 2c_3 + 2c_1(2 + c_2 + c_3), 0\}, \{2(1 + c_2), 1 + 2c_2, 2(2 + c_2 + c_3)\}\}$	
20 $mmmF$	7 m_y	9 $\{\{1, 0, 0\}, \{4 + c_2 + 3c_3 + 2c_1(2 + c_2 + c_3), 5 + c_2 + 3c_3 + 2c_1(2 + c_2 + c_3), 0\}, \{2(1 + c_2), 1 + 2c_2, 2(2 + c_2 + c_3)\}\}$	
20 $mmmF$	7 m_y	10 $\{\{1, 0, 0\}, \{1 + 2c_3 + c_1(3 + 2c_2 + 2c_3), 2(1 + c_3) + c_1(3 + 2c_2 + 2c_3), 0\}, \{2(1 + c_2), 1 + 2c_2, 3 + 2c_2 + 2c_3\}\}$	
20 $mmmF$	7 m_y	11 $\{\{1, 0, 0\}, \{2(1 + c_3) + c_1(3 + 2c_2 + 2c_3), 3 + 2c_3 + c_1(3 + 2c_2 + 2c_3), 0\}, \{1 + 2c_2, 2c_2, 3 + 2c_2 + 2c_3\}\}$	
20 $mmmF$	8 m_z	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{d_1, d_2, 1 + d_1 + d_2\}\}$	2
20 $mmmF$	8 m_z	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, c_1, 2 + c_1\}\}$	
20 $mmmF$	8 m_z	3 $\{\{1, 0, 0\}, \{1, 2(1 + c_1), 0\}, \{c_1, 0, 1 + c_1\}\}$	
20 $mmmF$	8 m_z	4 $\{\{1, 0, 0\}, \{1, 2(3 + d_1 + d_2), 0\}, \{5 + 2d_1 + 3d_2, 3 + d_1 + d_2, 6 + 2d_1 + 3d_2\}\}$	37
20 $mmmF$	8 m_z	5 $\{\{1, 0, 0\}, \{1, 2(2 + c_1), 0\}, \{5 + 3c_1 + 2(2 + c_1)d_1 + 2(2 + c_1)d_2, 2(2 + c_1)d_1, (2 + c_1)(3 + 2d_1 + 2d_2)\}\}$	28
20 $mmmF$	8 m_z	6 $\{\{1, 0, 0\}, \{1, 2(2 + c_1), 0\}, \{5 + 4d_1 + 2d_2 + c_1(3 + 2d_1 + d_2), (2 + c_1)(1 + 2d_1), (2 + c_1)(3 + 2d_1 + d_2)\}\}$	25
20 $mmmF$	8 m_z	7 $\{\{1, 0, 0\}, \{1, 3 + c_1, 0\}, \{2 + c_1 + (3 + c_1)d_1 + (3 + c_1)d_2, (3 + c_1)d_1, (3 + c_1)(1 + d_1 + d_2)\}\}$	2
20 $mmmF$	8 m_z	8 $\{\{1, 0, 0\}, \{1, 2(1 + d_1), 0\}, \{3 + 3d_1 + 2(1 + d_1)d_2 + d_3, (1 + d_1)(1 + 2d_2), 4 + 3d_1 + 2(1 + d_1)d_2 + d_3\}\}$	44
20 $mmmF$	8 m_z	9 $\{\{1, 0, 0\}, \{1, 2 + d_1, 0\}, \{2 + d_1 + (2 + d_1)d_2 + d_3, (2 + d_1)d_2, 3 + d_1 + (2 + d_1)d_2 + d_3\}\}$	43
20 $mmmF$	8 m_z	10 $\{\{1, 0, 0\}, \{1, 2(2 + d_1 + d_2), 0\}, \{4 + 2d_1 + 3d_2 + 2(2 + d_1 + d_2)d_3, (2 + d_1 + d_2)(1 + 2d_3), 5 + 2d_1 + 3d_2 + 2(2 + d_1 + d_2)d_3\}\}$	48
20 $mmmF$	8 m_z	11 $\{\{1, 0, 0\}, \{1, 2(3 + d_1 + d_2), 0\}, \{6 + 2d_1 + 3d_2 + 2(3 + d_1 + d_2)d_3, (3 + d_1 + d_2)(1 + 2d_3), 7 + 2d_1 + 3d_2 + 2(3 + d_1 + d_2)d_3\}\}$	49
20 $mmmF$	8 m_z	12 $\{\{1, 0, 0\}, \{1, 2(3 + d_1 + d_2), 0\}, \{5 + 2d_1 + 3d_2 + 2(3 + d_1 + d_2)(1 + d_3), (3 + d_1 + d_2)(3 + 2d_3), 6 + 2d_1 + 3d_2 + 2(3 + d_1 + d_2)(1 + d_3)\}\}$	50
20 $mmmF$	8 m_z	13 $\{\{1, 0, 0\}, \{1, 4 + 2d_1 + d_2, 0\}, \{2 + d_1 + d_2 + (4 + 2d_1 + d_2)(1 + d_3), (4 + 2d_1 + d_2)(1 + d_3), 3 + d_1 + d_2 + (4 + 2d_1 + d_2)(1 + d_3)\}\}$	45
20 $mmmF$	8 m_z	14 $\{\{1, 0, 0\}, \{1, 5 + 2d_1 + d_2, 0\}, \{2 + d_1 + d_2 + (5 + 2d_1 + d_2)(1 + d_3), (5 + 2d_1 + d_2)(1 + d_3), 3 + d_1 + d_2 + (5 + 2d_1 + d_2)(1 + d_3)\}\}$	46
20 $mmmF$	8 m_z	15 $\{\{1, 0, 0\}, \{1, 6 + 2d_1 + d_2, 0\}, \{2 + d_1 + d_2 + (6 + 2d_1 + d_2)(1 + d_3), (6 + 2d_1 + d_2)(1 + d_3), 3 + d_1 + d_2 + (6 + 2d_1 + d_2)(1 + d_3)\}\}$	47
20 $mmmF$	9 $2/m_x$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
20 $mmmF$	9 $2/m_x$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
20 $mmmF$	9 $2/m_x$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
20 $mmmF$	9 $2/m_x$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
20 $mmmF$	9 $2/m_x$	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
20 $mmmF$	10 $2/m_y$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	

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Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#	
20	$mmmF$	10 $2/m_y$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
20	$mmmF$	10 $2/m_y$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
20	$mmmF$	10 $2/m_y$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
20	$mmmF$	10 $2/m_y$	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
20	$mmmF$	11 $2/m_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
20	$mmmF$	11 $2/m_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
20	$mmmF$	11 $2/m_z$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
20	$mmmF$	11 $2/m_z$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
20	$mmmF$	11 $2/m_z$	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
20	$mmmF$	12 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
20	$mmmF$	12 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
20	$mmmF$	12 222	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
20	$mmmF$	12 222	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
20	$mmmF$	12 222	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
20	$mmmF$	13 $2_x mm$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
20	$mmmF$	13 $2_x mm$	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, c_1, 2 + c_1\}\}$	
20	$mmmF$	13 $2_x mm$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, c_1, 1 + c_1\}\}$	
20	$mmmF$	13 $2_x mm$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, c_1, 2 + 2c_1\}\}$	
20	$mmmF$	14 $m2_y m$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{c_1, 0, 1 + c_1\}\}$	
20	$mmmF$	14 $m2_y m$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{c_1, 1 + c_1, 2 + 2c_1\}\}$	
20	$mmmF$	14 $m2_y m$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{c_1, 0, 1 + c_1\}\}$	
20	$mmmF$	15 $mm2_z$	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 0, 2\}\}$	
20	$mmmF$	15 $mm2_z$	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 1, 2\}\}$	
20	$mmmF$	15 $mm2_z$	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
20	$mmmF$	16 mmm	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
20	$mmmF$	16 mmm	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
20	$mmmF$	16 mmm	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
20	$mmmF$	16 mmm	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
20	$mmmF$	16 mmm	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
21	$mmmI$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21	$mmmI$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
21	$mmmI$	2 $\bar{1}$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
21	$mmmI$	2 $\bar{1}$	4 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
21	$mmmI$	2 $\bar{1}$	5 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
21	$mmmI$	2 $\bar{1}$	6 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
21	$mmmI$	3 2_x	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21	$mmmI$	3 2_x	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + 2c_1, 3 + 4c_1, 4(1 + c_1)\}\}$	
21	$mmmI$	3 2_x	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1 + c_1, 2 + c_1\}\}$	
21	$mmmI$	3 2_x	4 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
21	$mmmI$	3 2_x	5 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{2, 3 + 2c_1, 2(2 + c_1)\}\}$	
21	$mmmI$	4 2_y	1 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
21	$mmmI$	4 2_y	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21	$mmmI$	4 2_y	3 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{3 + 2c_1, 2, 2(2 + c_1)\}\}$	
21	$mmmI$	4 2_y	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + 4c_1, 3 + 2c_1, 4(1 + c_1)\}\}$	
21	$mmmI$	4 2_y	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1, 2 + c_1\}\}$	
21	$mmmI$	5 2_z	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
21	$mmmI$	5 2_z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21	$mmmI$	5 2_z	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{2, 2, 2(2 + c_1)\}\}$	
21	$mmmI$	5 2_z	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + 2c_1, 3 + 2c_1, 4(1 + c_1)\}\}$	
21	$mmmI$	5 2_z	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2 + c_1\}\}$	
21	$mmmI$	6 m_x	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21	$mmmI$	6 m_x	2 $\{\{2 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2 + c_1\}\}$	
21	$mmmI$	6 m_x	3 $\{\{2 + c_1, 0, 0\}, \{0, 1, 0\}, \{(2 + c_1)(1 + c_2), 1, (2 + c_1)(2 + c_2)\}\}$	
21	$mmmI$	6 m_x	4 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{(1 + c_1)(1 + d_1), 1, (1 + c_1)(3 + d_1 + d_2)\}\}$	10
21	$mmmI$	6 m_x	5 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1, 2(1 + c_1)\}\}$	
21	$mmmI$	6 m_x	6 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1, (1 + c_1)(3 + c_2)\}\}$	
21	$mmmI$	6 m_x	7 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{(1 + c_1)(2 + d_1), 1, (1 + c_1)(3 + d_1 + d_2)\}\}$	13
21	$mmmI$	7 m_y	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21	$mmmI$	7 m_y	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 3\}\}$	
21	$mmmI$	7 m_y	3 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 2, 8\}\}$	
21	$mmmI$	7 m_y	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 4 + c_1\}\}$	
21	$mmmI$	7 m_y	5 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, 0, 2 + c_1\}\}$	
21	$mmmI$	7 m_y	6 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, 2 + c_1, 3(2 + c_1)\}\}$	
21	$mmmI$	7 m_y	7 $\{\{1, 0, 0\}, \{0, 3 + c_1, 0\}, \{1, 3 + c_1, 4(3 + c_1)\}\}$	
21	$mmmI$	7 m_y	8 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, (2 + c_1)(1 + c_2), (2 + c_1)(2 + c_2)\}\}$	
21	$mmmI$	7 m_y	9 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 2 + d_1, 5 + d_1 + d_2\}\}$	21
21	$mmmI$	7 m_y	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 2(1 + d_1), 2(5 + d_1 + d_2)\}\}$	20
21	$mmmI$	7 m_y	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 2(2 + d_1), 2(5 + d_1 + d_2)\}\}$	21
21	$mmmI$	7 m_y	12 $\{\{1, 0, 0\}, \{0, 3 + c_1, 0\}, \{1, (3 + c_1)(1 + d_1), (3 + c_1)(5 + d_1 + d_2)\}\}$	20
21	$mmmI$	7 m_y	13 $\{\{1, 0, 0\}, \{0, 3 + c_1, 0\}, \{1, (3 + c_1)(2 + d_1), (3 + c_1)(5 + d_1 + d_2)\}\}$	21
21	$mmmI$	7 m_y	14 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 2 + c_1, 3 + c_1\}\}$	
21	$mmmI$	7 m_y	15 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1, 1 + c_1, 2(1 + c_1)\}\}$	
21	$mmmI$	7 m_y	16 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1, 1 + c_1, (1 + c_1)(3 + c_2)\}\}$	
21	$mmmI$	7 m_y	17 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, (2 + c_1)(2 + c_2), (2 + c_1)(3 + c_2)\}\}$	
21	$mmmI$	7 m_y	18 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 3 + d_1, 5 + d_1 + d_2\}\}$	22
21	$mmmI$	7 m_y	19 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, (2 + c_1)(2 + d_1), (2 + c_1)(5 + d_1 + d_2)\}\}$	21
21	$mmmI$	7 m_y	20 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, (2 + c_1)(3 + d_1), (2 + c_1)(5 + d_1 + d_2)\}\}$	22

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
21 $mmmI$	$8 m_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	5
21 $mmmI$	$8 m_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + d_1, 1 + d_2, 2 + d_1 + d_2\}\}$	
21 $mmmI$	$8 m_z$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
21 $mmmI$	$8 m_z$	4 $\{\{1, 0, 0\}, \{1, 3, 0\}, \{0, 3, 6\}\}$	
21 $mmmI$	$8 m_z$	5 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 0, 2 + c_1\}\}$	
21 $mmmI$	$8 m_z$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 2, 2(2 + c_1)\}\}$	
21 $mmmI$	$8 m_z$	7 $\{\{1, 0, 0\}, \{1, 4 + c_1, 0\}, \{0, 4 + c_1, 2(4 + c_1)\}\}$	
21 $mmmI$	$8 m_z$	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 2(2 + d_1), 2(3 + d_1 + d_2)\}\}$	
21 $mmmI$	$8 m_z$	9 $\{\{1, 0, 0\}, \{1, 3, 0\}, \{0, 3(1 + d_1), 3(3 + d_1 + d_2)\}\}$	
21 $mmmI$	$8 m_z$	10 $\{\{1, 0, 0\}, \{1, 3, 0\}, \{0, 3(2 + d_1), 3(3 + d_1 + d_2)\}\}$	
21 $mmmI$	$8 m_z$	11 $\{\{1, 0, 0\}, \{1, 4 + c_1, 0\}, \{0, (4 + c_1)(1 + d_1), (4 + c_1)(3 + d_1 + d_2)\}\}$	
21 $mmmI$	$8 m_z$	12 $\{\{1, 0, 0\}, \{1, 4 + c_1, 0\}, \{0, (4 + c_1)(2 + d_1), (4 + c_1)(3 + d_1 + d_2)\}\}$	
21 $mmmI$	$9 2/m_x$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	13
21 $mmmI$	$9 2/m_x$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21 $mmmI$	$9 2/m_x$	3 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
21 $mmmI$	$10 2/m_y$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
21 $mmmI$	$10 2/m_y$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21 $mmmI$	$10 2/m_y$	3 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
21 $mmmI$	$11 2/m_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21 $mmmI$	$11 2/m_z$	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
21 $mmmI$	$11 2/m_z$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
21 $mmmI$	$12 222$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
21 $mmmI$	$12 222$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
21 $mmmI$	$12 222$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21 $mmmI$	$12 222$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
21 $mmmI$	$12 222$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
21 $mmmI$	$12 222$	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21 $mmmI$	$13 2_x mm$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21 $mmmI$	$13 2_x mm$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1 + c_1, 2 + c_1\}\}$	
21 $mmmI$	$14 m^2_y m$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21 $mmmI$	$14 m^2_y m$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1, 2 + c_1\}\}$	
21 $mmmI$	$15 mm2_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21 $mmmI$	$15 mm2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2 + c_1\}\}$	
21 $mmmI$	$16 mmm$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
21 $mmmI$	$16 mmm$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
22 $4P$	$2 2_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
22 $4P$	$2 2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
22 $4P$	$2 2_z$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
22 $4P$	$2 2_z$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
22 $4P$	$2 2_z$	5 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
22 $4P$	$3 4$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
22 $4P$	$3 4$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
22 $4P$	$3 4$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
23 $4I$	$2 2_z$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
23 $4I$	$2 2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
23 $4I$	$2 2_z$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{2, 2, 2(2 + c_1)\}\}$	
23 $4I$	$2 2_z$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + 2c_1, 3 + 2c_1, 4(1 + c_1)\}\}$	
23 $4I$	$2 2_z$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2 + c_1\}\}$	
23 $4I$	$3 4$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
23 $4I$	$3 4$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2 + c_1\}\}$	
24 $4P$	$2 2_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
24 $4P$	$2 2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
24 $4P$	$2 2_z$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
24 $4P$	$2 2_z$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
24 $4P$	$2 2_z$	5 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
24 $4P$	$3 \bar{4}$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
24 $4P$	$3 \bar{4}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
24 $4P$	$3 \bar{4}$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
24 $4P$	$3 \bar{4}$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
24 $4P$	$3 \bar{4}$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
25 $4I$	$2 2_z$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
25 $4I$	$2 2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
25 $4I$	$2 2_z$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{2, 2, 2(2 + c_1)\}\}$	
25 $4I$	$2 2_z$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + 2c_1, 3 + 2c_1, 4(1 + c_1)\}\}$	
25 $4I$	$2 2_z$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2 + c_1\}\}$	
25 $4I$	$3 \bar{4}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
25 $4I$	$3 \bar{4}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
25 $4I$	$3 \bar{4}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
25 $4I$	$3 \bar{4}$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
25 $4I$	$3 \bar{4}$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
25 $4I$	$3 \bar{4}$	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
26 $4/mP$	$2 \bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
26 $4/mP$	$2 \bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
26 $4/mP$	$2 \bar{1}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
26 $4/mP$	$2 \bar{1}$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
26 $4/mP$	$2 \bar{1}$	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
26 $4/mP$	$2 \bar{1}$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
26 4/mP	2 $\bar{1}$	7 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1}}	
26 4/mP	2 $\bar{1}$	8 {{2, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
26 4/mP	3 2 _z	1 {{1, 0, 0}, {0, 1, 0}, {1 + c ₁ , 1 + c ₁ , 2 + 2c ₁ }}	
26 4/mP	3 2 _z	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c ₁ }}	
26 4/mP	3 2 _z	3 {{1, 0, 0}, {1, 2, 0}, {1 + c ₁ , 0, 2 + 2c ₁ }}	
26 4/mP	3 2 _z	4 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c ₁ }}	
26 4/mP	3 2 _z	5 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1 + c ₁ }}	
26 4/mP	4 m _z	1 {{1 + c ₁ , 0, 0}, {0, 1 + c ₁ , 0}, {0, 0, 1}}	
26 4/mP	4 m _z	2 {{1 + c ₁ , 0, 0}, {(1 + c ₁)(1 + d ₁), (1 + c ₁)(2 + d ₁ + d ₂), 0}, {0, 0, 1}}	7
26 4/mP	4 m _z	3 {{1 + c ₁ , 0, 0}, {0, 1 + c ₁ , 0}, {0, 0, 2}}	
26 4/mP	4 m _z	4 {{1 + c ₁ , 0, 0}, {(1 + c ₁)(1 + d ₁), (1 + c ₁)(2 + d ₁ + d ₂), 0}, {0, 0, 2}}	7
26 4/mP	4 m _z	5 {{1 + c ₁ , 0, 0}, {(1 + c ₁)(1 + 2d ₁), (1 + c ₁)(2 + 2d ₁ + d ₂), 0}, {0, 1, 2}}	23
26 4/mP	4 m _z	6 {{1 + c ₁ , 0, 0}, {(1 + c ₁)(1 + 2d ₁), 2(1 + c ₁)(1 + d ₁ + d ₂), 0}, {1, 0, 2}}	3
26 4/mP	4 m _z	7 {{1 + c ₁ , 0, 0}, {0, 1 + c ₁ , 0}, {1, 1, 2}}	
26 4/mP	4 m _z	8 {{1 + c ₁ , 0, 0}, {(1 + c ₁)d ₁ , (1 + c ₁)(3 + d ₁ + 2d ₂), 0}, {1, 1, 2}}	35
26 4/mP	5 2/m _z	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
26 4/mP	5 2/m _z	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
26 4/mP	5 2/m _z	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
26 4/mP	5 2/m _z	4 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
26 4/mP	5 2/m _z	5 {{1, 0, 0}, {1, 2, 0}, {1, 0, 2}}	
26 4/mP	5 2/m _z	6 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
26 4/mP	5 2/m _z	7 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1}}	
26 4/mP	5 2/m _z	8 {{2, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
26 4/mP	6 4	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c ₁ }}	
26 4/mP	6 4	2 {{1, 0, 0}, {0, 1, 0}, {1 + c ₁ , 1 + c ₁ , 2 + 2c ₁ }}	
26 4/mP	6 4	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c ₁ }}	
26 4/mP	7 4	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
26 4/mP	7 4	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
26 4/mP	7 4	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
26 4/mP	7 4	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
26 4/mP	7 4	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
26 4/mP	8 4/m	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
26 4/mP	8 4/m	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
26 4/mP	8 4/m	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
26 4/mP	8 4/m	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
26 4/mP	8 4/m	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
27 4/mI	2 $\bar{1}$	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
27 4/mI	2 $\bar{1}$	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
27 4/mI	2 $\bar{1}$	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
27 4/mI	2 $\bar{1}$	4 {{2, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
27 4/mI	3 2 _z	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
27 4/mI	3 2 _z	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
27 4/mI	3 2 _z	3 {{1, 0, 0}, {1, 2, 0}, {2, 2, 2(2 + c ₁)}}	
27 4/mI	3 2 _z	4 {{1, 0, 0}, {0, 1, 0}, {3 + 2c ₁ , 3 + 2c ₁ , 4(1 + c ₁)}}	
27 4/mI	3 2 _z	5 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c ₁ }}	
27 4/mI	4 m _z	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
27 4/mI	4 m _z	2 {{1, 0, 0}, {0, 1, 0}, {1 + d ₁ , 1 + d ₂ , 2 + d ₁ + d ₂ }}	7
27 4/mI	4 m _z	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
27 4/mI	4 m _z	4 {{1, 0, 0}, {1, 2, 0}, {0, 2, 4}}	
27 4/mI	4 m _z	5 {{1, 0, 0}, {1, 3, 0}, {0, 3, 6}}	
27 4/mI	4 m _z	6 {{1, 0, 0}, {1, 2 + c ₁ , 0}, {0, 0, 2 + c ₁ }}	
27 4/mI	4 m _z	7 {{1, 0, 0}, {1, 4 + c ₁ , 0}, {0, 4 + c ₁ , 2(4 + c ₁)}}	
27 4/mI	4 m _z	8 {{1, 0, 0}, {1, 2, 0}, {0, 2(2 + d ₁), 2(3 + d ₁ + d ₂)}}	14
27 4/mI	4 m _z	9 {{1, 0, 0}, {1, 3, 0}, {0, 3(1 + d ₁), 3(3 + d ₁ + d ₂)}}	11
27 4/mI	4 m _z	10 {{1, 0, 0}, {1, 3, 0}, {0, 3(2 + d ₁), 3(3 + d ₁ + d ₂)}}	14
27 4/mI	4 m _z	11 {{1, 0, 0}, {1, 4 + c ₁ , 0}, {0, (4 + c ₁)(1 + d ₁), (4 + c ₁)(3 + d ₁ + d ₂)}}	11
27 4/mI	4 m _z	12 {{1, 0, 0}, {1, 4 + c ₁ , 0}, {0, (4 + c ₁)(2 + d ₁), (4 + c ₁)(3 + d ₁ + d ₂)}}	14
27 4/mI	5 2/m _z	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
27 4/mI	5 2/m _z	2 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
27 4/mI	5 2/m _z	3 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
27 4/mI	6 4	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
27 4/mI	6 4	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c ₁ }}	
27 4/mI	7 4	1 {{1, 0, 0}, {0, 1, 0}, {3, 3, 4}}	
27 4/mI	7 4	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
27 4/mI	7 4	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
27 4/mI	7 4	4 {{1, 0, 0}, {0, 1, 0}, {3, 3, 4}}	
27 4/mI	7 4	5 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
27 4/mI	7 4	6 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
27 4/mI	8 4/m	1 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
27 4/mI	8 4/m	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
28 422P	2 2 _z	1 {{1, 0, 0}, {0, 1, 0}, {1 + c ₁ , 1 + c ₁ , 2 + 2c ₁ }}	
28 422P	2 2 _z	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c ₁ }}	
28 422P	2 2 _z	3 {{1, 0, 0}, {1, 2, 0}, {1 + c ₁ , 0, 2 + 2c ₁ }}	
28 422P	2 2 _z	4 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c ₁ }}	
28 422P	2 2 _z	5 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1 + c ₁ }}	
28 422P	3 222	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
28 422P	3 222	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
28 422P	3 222	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
28 422P	3 222	4 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
28 422P	3 222	5 {{1, 0, 0}, {1, 2, 0}, {1, 0, 2}}	
28 422P	3 222	6 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
28 422P	3 222	7 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1}}	
28 422P	3 222	8 {{2, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
28 422P	4 222 _d	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
28 422P	4 222 _d	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
28 422P	4 222 _d	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
28 422P	4 222 _d	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
28 422P	4 222 _d	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
28 422P	5 4	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c _{1}}}	
28 422P	5 4	2 {{1, 0, 0}, {0, 1, 0}, {1 + c _{1}, 1 + c_{1}, 2 + 2c_{1}}}}}	
28 422P	5 4	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
28 422P	6 422	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
28 422P	6 422	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
28 422P	6 422	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
28 422P	6 422	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
28 422P	6 422	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
29 422I	2 2 _z	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
29 422I	2 2 _z	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
29 422I	2 2 _z	3 {{1, 0, 0}, {1, 2, 0}, {2, 2, 2(2 + c _{1})}}}	
29 422I	2 2 _z	4 {{1, 0, 0}, {0, 1, 0}, {3 + 2c _{1}, 3 + 2c_{1}, 4(1 + c_{1})}}}}}	
29 422I	2 2 _z	5 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c _{1}}}	
29 422I	3 222	1 {{1, 0, 0}, {0, 1, 0}, {3, 3, 4}}	
29 422I	3 222	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
29 422I	3 222	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
29 422I	3 222	4 {{1, 0, 0}, {0, 1, 0}, {3, 3, 4}}	
29 422I	3 222	5 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
29 422I	3 222	6 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
29 422I	4 222 _d	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
29 422I	4 222 _d	2 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
29 422I	4 222 _d	3 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
29 422I	5 4	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
29 422I	5 4	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c _{1}}}	
29 422I	6 422	1 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
29 422I	6 422	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
30 4mmP	2 2 _z	1 {{1, 0, 0}, {0, 1, 0}, {1 + c _{1}, 1 + c_{1}, 2 + 2c_{1}}}}}	
30 4mmP	2 2 _z	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
30 4mmP	2 2 _z	3 {{1, 0, 0}, {1, 2, 0}, {1 + c _{1}, 0, 2 + 2c_{1}}}}	
30 4mmP	2 2 _z	4 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c _{1}}}	
30 4mmP	2 2 _z	5 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1 + c _{1}}}	
30 4mmP	3 mm2 _z	1 {{1, 0, 0}, {0, 1, 0}, {1 + c _{1}, 1 + c_{1}, 2 + 2c_{1}}}}}	
30 4mmP	3 mm2 _z	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
30 4mmP	3 mm2 _z	3 {{1, 0, 0}, {1, 2, 0}, {1 + c _{1}, 0, 2 + 2c_{1}}}}	
30 4mmP	3 mm2 _z	4 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c _{1}}}	
30 4mmP	3 mm2 _z	5 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1 + c _{1}}}	
30 4mmP	4 mm2 _d	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c _{1}}}	
30 4mmP	4 mm2 _d	2 {{1, 0, 0}, {0, 1, 0}, {1 + c _{1}, 1 + c_{1}, 2 + 2c_{1}}}}}	
30 4mmP	4 mm2 _d	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
30 4mmP	5 4	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c _{1}}}	
30 4mmP	5 4	2 {{1, 0, 0}, {0, 1, 0}, {1 + c _{1}, 1 + c_{1}, 2 + 2c_{1}}}}}	
30 4mmP	5 4	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
30 4mmP	6 4mm	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c _{1}}}	
30 4mmP	6 4mm	2 {{1, 0, 0}, {0, 1, 0}, {1 + c _{1}, 1 + c_{1}, 2 + 2c_{1}}}}}	
30 4mmP	6 4mm	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
31 4mmI	2 2 _z	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
31 4mmI	2 2 _z	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
31 4mmI	2 2 _z	3 {{1, 0, 0}, {1, 2, 0}, {2, 2, 2(2 + c _{1})}}}	
31 4mmI	2 2 _z	4 {{1, 0, 0}, {0, 1, 0}, {3 + 2c _{1}, 3 + 2c_{1}, 4(1 + c_{1})}}}}}	
31 4mmI	2 2 _z	5 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c _{1}}}	
31 4mmI	3 mm2 _z	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
31 4mmI	3 mm2 _z	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c _{1}}}	
31 4mmI	4 mm2 _d	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
31 4mmI	4 mm2 _d	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
31 4mmI	4 mm2 _d	3 {{1, 0, 0}, {1, 2, 0}, {2, 2, 2(2 + c _{1})}}}	
31 4mmI	4 mm2 _d	4 {{1, 0, 0}, {0, 1, 0}, {3 + 2c _{1}, 3 + 2c_{1}, 4(1 + c_{1})}}}}}	
31 4mmI	4 mm2 _d	5 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c _{1}}}	
31 4mmI	5 4	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
31 4mmI	5 4	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c _{1}}}	
31 4mmI	6 4mm	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
31 4mmI	6 4mm	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c _{1}}}	
32 42mP	2 2 _z	1 {{1, 0, 0}, {0, 1, 0}, {1 + c _{1}, 1 + c_{1}, 2 + 2c_{1}}}}}	
32 42mP	2 2 _z	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
32 42mP	2 2 _z	3 {{1, 0, 0}, {1, 2, 0}, {1 + c _{1}, 0, 2 + 2c_{1}}}}	
32 42mP	2 2 _z	4 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c _{1}}}	
32 42mP	2 2 _z	5 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1 + c _{1}}}	

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
32 $\bar{4}2mP$	3 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
32 $\bar{4}2mP$	3 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
32 $\bar{4}2mP$	3 222	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
32 $\bar{4}2mP$	3 222	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
32 $\bar{4}2mP$	3 222	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
32 $\bar{4}2mP$	3 222	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
32 $\bar{4}2mP$	3 222	7 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
32 $\bar{4}2mP$	3 222	8 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
32 $\bar{4}2mP$	4 $mm2_d$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
32 $\bar{4}2mP$	4 $mm2_d$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
32 $\bar{4}2mP$	4 $mm2_d$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
32 $\bar{4}2mP$	5 $\bar{4}$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
32 $\bar{4}2mP$	5 $\bar{4}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
32 $\bar{4}2mP$	5 $\bar{4}$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
32 $\bar{4}2mP$	5 $\bar{4}$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
32 $\bar{4}2mP$	5 $\bar{4}$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
32 $\bar{4}2mP$	6 $\bar{4}2m$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
32 $\bar{4}2mP$	6 $\bar{4}2m$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
32 $\bar{4}2mP$	6 $\bar{4}2m$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
32 $\bar{4}2mP$	6 $\bar{4}2m$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
32 $\bar{4}2mP$	6 $\bar{4}2m$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
33 $\bar{4}m2P$	2 2 _z	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
33 $\bar{4}m2P$	2 2 _z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
33 $\bar{4}m2P$	2 2 _z	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
33 $\bar{4}m2P$	2 2 _z	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
33 $\bar{4}m2P$	2 2 _z	5 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
33 $\bar{4}m2P$	3 222 _d	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
33 $\bar{4}m2P$	3 222 _d	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
33 $\bar{4}m2P$	3 222 _d	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
33 $\bar{4}m2P$	3 222 _d	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
33 $\bar{4}m2P$	3 222 _d	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
33 $\bar{4}m2P$	4 $mm2_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
33 $\bar{4}m2P$	4 $mm2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
33 $\bar{4}m2P$	4 $mm2_z$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
33 $\bar{4}m2P$	4 $mm2_z$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
33 $\bar{4}m2P$	4 $mm2_z$	5 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
33 $\bar{4}m2P$	5 $\bar{4}$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
33 $\bar{4}m2P$	5 $\bar{4}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
33 $\bar{4}m2P$	5 $\bar{4}$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
33 $\bar{4}m2P$	5 $\bar{4}$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
33 $\bar{4}m2P$	5 $\bar{4}$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
33 $\bar{4}m2P$	6 $\bar{4}m2$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
33 $\bar{4}m2P$	6 $\bar{4}m2$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
33 $\bar{4}m2P$	6 $\bar{4}m2$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
33 $\bar{4}m2P$	6 $\bar{4}m2$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
33 $\bar{4}m2P$	6 $\bar{4}m2$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
34 $\bar{4}m2I$	2 2 _z	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
34 $\bar{4}m2I$	2 2 _z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
34 $\bar{4}m2I$	2 2 _z	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{2, 2, 2(2 + c_1)\}\}$	
34 $\bar{4}m2I$	2 2 _z	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + 2c_1, 3 + 2c_1, 4(1 + c_1)\}\}$	
34 $\bar{4}m2I$	2 2 _z	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2 + c_1\}\}$	
34 $\bar{4}m2I$	3 222 _d	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
34 $\bar{4}m2I$	3 222 _d	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
34 $\bar{4}m2I$	3 222 _d	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
34 $\bar{4}m2I$	4 $mm2_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
34 $\bar{4}m2I$	4 $mm2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2 + c_1\}\}$	
34 $\bar{4}m2I$	5 $\bar{4}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
34 $\bar{4}m2I$	5 $\bar{4}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
34 $\bar{4}m2I$	5 $\bar{4}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
34 $\bar{4}m2I$	5 $\bar{4}$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
34 $\bar{4}m2I$	5 $\bar{4}$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
34 $\bar{4}m2I$	5 $\bar{4}$	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
34 $\bar{4}m2I$	6 $\bar{4}m2$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
34 $\bar{4}m2I$	6 $\bar{4}m2$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
35 $\bar{4}2mI$	2 2 _z	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
35 $\bar{4}2mI$	2 2 _z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
35 $\bar{4}2mI$	2 2 _z	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{2, 2, 2(2 + c_1)\}\}$	
35 $\bar{4}2mI$	2 2 _z	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + 2c_1, 3 + 2c_1, 4(1 + c_1)\}\}$	
35 $\bar{4}2mI$	2 2 _z	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2 + c_1\}\}$	
35 $\bar{4}2mI$	3 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
35 $\bar{4}2mI$	3 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
35 $\bar{4}2mI$	3 222	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
35 $\bar{4}2mI$	3 222	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
35 $\bar{4}2mI$	3 222	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
35 $\bar{4}2mI$	3 222	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
35 $\bar{4}2mI$	4 $mm2_d$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
35 $\bar{4}2mI$	4 $mm2_d$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	

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Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
35 $\bar{4}2mI$	4 $mm2_d$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{2, 2, 2(2 + c_1)\}\}$	
35 $\bar{4}2mI$	4 $mm2_d$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + 2c_1, 3 + 2c_1, 4(1 + c_1)\}\}$	
35 $\bar{4}2mI$	4 $mm2_d$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2 + c_1\}\}$	
35 $\bar{4}2mI$	5 $\bar{4}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
35 $\bar{4}2mI$	5 $\bar{4}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
35 $\bar{4}2mI$	5 $\bar{4}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
35 $\bar{4}2mI$	5 $\bar{4}$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
35 $\bar{4}2mI$	5 $\bar{4}$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
35 $\bar{4}2mI$	5 $\bar{4}$	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
35 $\bar{4}2mI$	6 $\bar{4}2m$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
35 $\bar{4}2mI$	6 $\bar{4}2m$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
35 $\bar{4}2mI$	6 $\bar{4}2m$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
35 $\bar{4}2mI$	6 $\bar{4}2m$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
35 $\bar{4}2mI$	6 $\bar{4}2m$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
35 $\bar{4}2mI$	6 $\bar{4}2m$	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
36 $4/mmmP$	2 $\bar{1}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	2 $\bar{1}$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	2 $\bar{1}$	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
36 $4/mmmP$	2 $\bar{1}$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	2 $\bar{1}$	7 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	2 $\bar{1}$	8 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	3 2_z	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
36 $4/mmmP$	3 2_z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
36 $4/mmmP$	3 2_z	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
36 $4/mmmP$	3 2_z	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
36 $4/mmmP$	3 2_z	5 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
36 $4/mmmP$	4 m_z	1 $\{\{2(1 + c_1), 0, 0\}, \{0, 2(1 + c_1), 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	4 m_z	2 $\{\{2(1 + c_1), 0, 0\}, \{2(1 + c_1), 4(1 + c_1), 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	4 m_z	3 $\{\{1 + 2c_1, 0, 0\}, \{0, 1 + 2c_1, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	4 m_z	4 $\{\{1 + 2c_1, 0, 0\}, \{1 + 2c_1, 2 + 4c_1, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	4 m_z	5 $\{\{2(1 + c_1), 0, 0\}, \{2(1 + c_1)(2 + d_1), 4(1 + c_1)(2 + d_1), 0\}, \{0, 0, 1\}\}$	1
36 $4/mmmP$	4 m_z	6 $\{\{1 + 2c_1, 0, 0\}, \{(1 + 2c_1)(2 + d_1), 2(1 + 2c_1)(2 + d_1), 0\}, \{0, 0, 1\}\}$	1
36 $4/mmmP$	4 m_z	7 $\{\{2(1 + c_1), 0, 0\}, \{0, 2(1 + c_1), 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	4 m_z	8 $\{\{2(1 + c_1), 0, 0\}, \{2(1 + c_1), 4(1 + c_1), 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	4 m_z	9 $\{\{1 + 2c_1, 0, 0\}, \{0, 1 + 2c_1, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	4 m_z	10 $\{\{1 + 2c_1, 0, 0\}, \{1 + 2c_1, 2 + 4c_1, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	4 m_z	11 $\{\{2(1 + c_1), 0, 0\}, \{2(1 + c_1)(2 + d_1), 4(1 + c_1)(2 + d_1), 0\}, \{0, 0, 2\}\}$	1
36 $4/mmmP$	4 m_z	12 $\{\{1 + 2c_1, 0, 0\}, \{(1 + 2c_1)(2 + d_1), 2(1 + 2c_1)(2 + d_1), 0\}, \{0, 0, 2\}\}$	1
36 $4/mmmP$	4 m_z	13 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
36 $4/mmmP$	4 m_z	14 $\{\{2 + c_1, 0, 0\}, \{2 + c_1, 2(2 + c_1), 0\}, \{1, 0, 2\}\}$	
36 $4/mmmP$	4 m_z	15 $\{\{1, 0, 0\}, \{2 + d_1, 2(2 + d_1), 0\}, \{1, 0, 2\}\}$	1
36 $4/mmmP$	4 m_z	16 $\{\{1 + c_1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1, 1, 2\}\}$	
36 $4/mmmP$	5 $2/m_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	5 $2/m_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
36 $4/mmmP$	5 $2/m_z$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	5 $2/m_z$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	5 $2/m_z$	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
36 $4/mmmP$	5 $2/m_z$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	5 $2/m_z$	7 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	5 $2/m_z$	8 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	6 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	6 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
36 $4/mmmP$	6 222	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	6 222	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	6 222	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
36 $4/mmmP$	6 222	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	6 222	7 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	6 222	8 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	7 222_d	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	7 222_d	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	7 222_d	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	7 222_d	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
36 $4/mmmP$	7 222_d	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	8 $mm2_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
36 $4/mmmP$	8 $mm2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
36 $4/mmmP$	8 $mm2_z$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
36 $4/mmmP$	8 $mm2_z$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
36 $4/mmmP$	8 $mm2_z$	5 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
36 $4/mmmP$	9 $mm2_d$	1 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
36 $4/mmmP$	9 $mm2_d$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
36 $4/mmmP$	9 $mm2_d$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
36 $4/mmmP$	10 mmm	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
36 $4/mmmP$	10 mmm	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
36 $4/mmmP$	10 mmm	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
36 $4/mmmP$	10 mmm	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	

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Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
36 4/mmmP	10 mmm	5 {{1, 0, 0}, {1, 2, 0}, {1, 0, 2}}	
36 4/mmmP	10 mmm	6 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
36 4/mmmP	10 mmm	7 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1}}	
36 4/mmmP	10 mmm	8 {{2, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
36 4/mmmP	11 mmm _d	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
36 4/mmmP	11 mmm _d	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
36 4/mmmP	11 mmm _d	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
36 4/mmmP	11 mmm _d	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
36 4/mmmP	11 mmm _d	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
36 4/mmmP	12 4	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c _{1}}}	
36 4/mmmP	12 4	2 {{1, 0, 0}, {0, 1, 0}, {1 + c _{1}, 1 + c_{1}, 2 + 2c_{1}}}}}	
36 4/mmmP	12 4	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
36 4/mmmP	13 $\bar{4}$	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
36 4/mmmP	13 $\bar{4}$	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
36 4/mmmP	13 $\bar{4}$	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
36 4/mmmP	13 $\bar{4}$	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
36 4/mmmP	13 $\bar{4}$	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
36 4/mmmP	14 4/m	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
36 4/mmmP	14 4/m	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
36 4/mmmP	14 4/m	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
36 4/mmmP	14 4/m	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
36 4/mmmP	14 4/m	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
36 4/mmmP	15 422	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
36 4/mmmP	15 422	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
36 4/mmmP	15 422	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
36 4/mmmP	15 422	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
36 4/mmmP	15 422	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
36 4/mmmP	16 4mm	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1 + c _{1}}}	
36 4/mmmP	16 4mm	2 {{1, 0, 0}, {0, 1, 0}, {1 + c _{1}, 1 + c_{1}, 2 + 2c_{1}}}}}	
36 4/mmmP	16 4mm	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c _{1}}}	
36 4/mmmP	17 $\bar{4}2m$	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
36 4/mmmP	17 $\bar{4}2m$	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
36 4/mmmP	17 $\bar{4}2m$	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
36 4/mmmP	17 $\bar{4}2m$	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
36 4/mmmP	17 $\bar{4}2m$	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
36 4/mmmP	18 $\bar{4}m2$	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
36 4/mmmP	18 $\bar{4}m2$	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
36 4/mmmP	18 $\bar{4}m2$	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
36 4/mmmP	18 $\bar{4}m2$	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
36 4/mmmP	18 $\bar{4}m2$	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
36 4/mmmP	19 4/mmm	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 1}}	
36 4/mmmP	19 4/mmm	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
36 4/mmmP	19 4/mmm	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
36 4/mmmP	19 4/mmm	4 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
36 4/mmmP	19 4/mmm	5 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
37 4/mmmI	2 $\bar{1}$	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	2 $\bar{1}$	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	2 $\bar{1}$	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
37 4/mmmI	2 $\bar{1}$	4 {{2, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
37 4/mmmI	3 2 _z	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
37 4/mmmI	3 2 _z	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	3 2 _z	3 {{1, 0, 0}, {1, 2, 0}, {2, 2, 2(2 + c _{1})}}}	
37 4/mmmI	3 2 _z	4 {{1, 0, 0}, {0, 1, 0}, {3 + 2c _{1}, 3 + 2c_{1}, 4(1 + c_{1})}}}}}	
37 4/mmmI	3 2 _z	5 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c _{1}}}	
37 4/mmmI	4 m _z	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	4 m _z	2 {{1, 0, 0}, {0, 1, 0}, {1 + d _{1}, 1 + d_{2}, 2 + d_{1} + d_{2}}}}}}	
37 4/mmmI	4 m _z	3 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
37 4/mmmI	4 m _z	4 {{1, 0, 0}, {1, 2, 0}, {0, 2, 4}}	
37 4/mmmI	4 m _z	5 {{1, 0, 0}, {1, 3, 0}, {0, 3, 6}}	
37 4/mmmI	4 m _z	6 {{1, 0, 0}, {1, 2 + c _{1}, 0}, {0, 0, 2 + c_{1}}}}	
37 4/mmmI	4 m _z	7 {{1, 0, 0}, {1, 4 + c _{1}, 0}, {0, 4 + c_{1}, 2(4 + c_{1})}}}}}	
37 4/mmmI	4 m _z	8 {{1, 0, 0}, {1, 2, 0}, {0, 2(2 + d _{1}), 2(3 + d_{1} + d_{2})}}}}}	
37 4/mmmI	4 m _z	9 {{1, 0, 0}, {1, 3, 0}, {0, 3(1 + d _{1}), 3(3 + d_{1} + d_{2})}}}}}	
37 4/mmmI	4 m _z	10 {{1, 0, 0}, {1, 3, 0}, {0, 3(2 + d _{1}), 3(3 + d_{1} + d_{2})}}}}}	
37 4/mmmI	4 m _z	11 {{1, 0, 0}, {1, 4 + c _{1}, 0}, {0, (4 + c_{1})(1 + d_{1}), (4 + c_{1})(3 + d_{1} + d_{2})}}}}}}}}	
37 4/mmmI	4 m _z	12 {{1, 0, 0}, {1, 4 + c _{1}, 0}, {0, (4 + c_{1})(2 + d_{1}), (4 + c_{1})(3 + d_{1} + d_{2})}}}}}}}}	
37 4/mmmI	5 2/m _z	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	5 2/m _z	2 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
37 4/mmmI	5 2/m _z	3 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	6 222	1 {{1, 0, 0}, {0, 1, 0}, {3, 3, 4}}	
37 4/mmmI	6 222	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	6 222	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	6 222	4 {{1, 0, 0}, {0, 1, 0}, {3, 3, 4}}	
37 4/mmmI	6 222	5 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	6 222	6 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	7 222 _d	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	7 222 _d	2 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	

31

34

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34

33

34

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
37 4/mmmI	7 222 _d	3 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	8 mm2 _z	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	8 mm2 _z	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c ₁ }}	
37 4/mmmI	9 mm2 _d	1 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
37 4/mmmI	9 mm2 _d	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	9 mm2 _d	3 {{1, 0, 0}, {1, 2, 0}, {2, 2, 2(2 + c ₁)}}	
37 4/mmmI	9 mm2 _d	4 {{1, 0, 0}, {0, 1, 0}, {3 + 2c ₁ , 3 + 2c ₁ , 4(1 + c ₁)}}	
37 4/mmmI	9 mm2 _d	5 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c ₁ }}	
37 4/mmmI	10 mmm	1 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	10 mmm	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	11 mmm _d	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	11 mmm _d	2 {{1, 0, 0}, {1, 2, 0}, {0, 0, 2}}	
37 4/mmmI	11 mmm _d	3 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	12 4	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	12 4	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c ₁ }}	
37 4/mmmI	13 4	1 {{1, 0, 0}, {0, 1, 0}, {3, 3, 4}}	
37 4/mmmI	13 4	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	13 4	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	13 4	4 {{1, 0, 0}, {0, 1, 0}, {3, 3, 4}}	
37 4/mmmI	13 4	5 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	13 4	6 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	14 4/m	1 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	14 4/m	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	15 422	1 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	15 422	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	16 4mm	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	16 4mm	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2 + c ₁ }}	
37 4/mmmI	17 42m	1 {{1, 0, 0}, {0, 1, 0}, {3, 3, 4}}	
37 4/mmmI	17 42m	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	17 42m	3 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	17 42m	4 {{1, 0, 0}, {0, 1, 0}, {3, 3, 4}}	
37 4/mmmI	17 42m	5 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	17 42m	6 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	18 4m2	1 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	18 4m2	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
37 4/mmmI	19 4/mmm	1 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
37 4/mmmI	19 4/mmm	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
38 3P	2 3	1 {{1, 0, 0}, {2, 3, 0}, {0, 0, 1 + c ₁ }}	
38 3P	2 3	2 {{1, 0, 0}, {0, 1, 0}, {2 + 2c ₁ , 2 + 2c ₁ , 3 + 3c ₁ }}	
38 3P	2 3	3 {{1, 0, 0}, {0, 1, 0}, {1 + c ₁ , 1 + c ₁ , 3 + 3c ₁ }}	
38 3P	2 3	4 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c ₁ }}	
39 3R	2 3	1 {{1, 0, 0}, {0, 1, 0}, {c ₁ , c ₁ , 1 + c ₁ }}	
40 3P	2 1	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
40 3P	2 1	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
40 3P	2 1	3 {{2, 0, 0}, {0, 2, 0}, {0, 0, 1}}	
40 3P	2 1	4 {{2, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
40 3P	3 3	1 {{1, 0, 0}, {2, 3, 0}, {0, 0, 1 + c ₁ }}	
40 3P	3 3	2 {{1, 0, 0}, {0, 1, 0}, {2 + 2c ₁ , 2 + 2c ₁ , 3 + 3c ₁ }}	
40 3P	3 3	3 {{1, 0, 0}, {0, 1, 0}, {1 + c ₁ , 1 + c ₁ , 3 + 3c ₁ }}	
40 3P	3 3	4 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c ₁ }}	
40 3P	4 3	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
40 3P	4 3	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
41 3R	2 1	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
41 3R	2 1	2 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
41 3R	2 1	3 {{1, 0, 0}, {1, 2, 0}, {1, 0, 2}}	
41 3R	2 1	4 {{2, 0, 0}, {0, 2, 0}, {0, 0, 2}}	
41 3R	3 3	1 {{1, 0, 0}, {0, 1, 0}, {c ₁ , c ₁ , 1 + c ₁ }}	
41 3R	4 3	1 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
41 3R	4 3	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
42 312P	2 3	1 {{1, 0, 0}, {2, 3, 0}, {0, 0, 1 + c ₁ }}	
42 312P	2 3	2 {{1, 0, 0}, {0, 1, 0}, {2 + 2c ₁ , 2 + 2c ₁ , 3 + 3c ₁ }}	
42 312P	2 3	3 {{1, 0, 0}, {0, 1, 0}, {1 + c ₁ , 1 + c ₁ , 3 + 3c ₁ }}	
42 312P	2 3	4 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c ₁ }}	
42 312P	3 312	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
42 312P	3 312	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
43 321P	2 3	1 {{1, 0, 0}, {2, 3, 0}, {0, 0, 1 + c ₁ }}	
43 321P	2 3	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c ₁ }}	
43 321P	3 321	1 {{1, 0, 0}, {2, 3, 0}, {0, 0, 1}}	
43 321P	3 321	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
43 321P	3 321	3 {{1, 0, 0}, {2, 3, 0}, {0, 0, 2}}	
43 321P	3 321	4 {{1, 0, 0}, {0, 1, 0}, {0, 0, 2}}	
44 32R	2 3	1 {{1, 0, 0}, {0, 1, 0}, {c ₁ , c ₁ , 1 + c ₁ }}	
44 32R	3 321	1 {{1, 0, 0}, {0, 1, 0}, {1, 1, 2}}	
44 32R	3 321	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}	
45 3m1P	2 3	1 {{1, 0, 0}, {2, 3, 0}, {0, 0, 1 + c ₁ }}	
45 3m1P	2 3	2 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c ₁ }}	
45 3m1P	3 3m1	1 {{1, 0, 0}, {0, 1, 0}, {0, 0, 1 + c ₁ }}	

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
46 $\bar{3}1mP$	2 3	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
46 $\bar{3}1mP$	2 3	2 $\{(1, 0, 0), \{0, 1, 0\}, \{2 + 2c_1, 2 + 2c_1, 3 + 3c_1\}\}$	
46 $\bar{3}1mP$	2 3	3 $\{(1, 0, 0), \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 3 + 3c_1\}\}$	
46 $\bar{3}1mP$	2 3	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
46 $\bar{3}1mP$	3 $\bar{3}1m$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
46 $\bar{3}1mP$	3 $\bar{3}1m$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{2 + 2c_1, 2 + 2c_1, 3 + 3c_1\}\}$	
46 $\bar{3}1mP$	3 $\bar{3}1m$	3 $\{(1, 0, 0), \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 3 + 3c_1\}\}$	
46 $\bar{3}1mP$	3 $\bar{3}1m$	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
47 $\bar{3}mR$	2 3	1 $\{(1, 0, 0), \{0, 1, 0\}, \{c_1, c_1, 1 + c_1\}\}$	
47 $\bar{3}mR$	3 $\bar{3}m1$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{c_1, c_1, 1 + c_1\}\}$	
48 $\bar{3}1mP$	2 $\bar{1}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
48 $\bar{3}1mP$	2 $\bar{1}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
48 $\bar{3}1mP$	2 $\bar{1}$	3 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 1\}\}$	
48 $\bar{3}1mP$	2 $\bar{1}$	4 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 2\}\}$	
48 $\bar{3}1mP$	3 3	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
48 $\bar{3}1mP$	3 3	2 $\{(1, 0, 0), \{0, 1, 0\}, \{2 + 2c_1, 2 + 2c_1, 3 + 3c_1\}\}$	
48 $\bar{3}1mP$	3 3	3 $\{(1, 0, 0), \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 3 + 3c_1\}\}$	
48 $\bar{3}1mP$	3 3	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
48 $\bar{3}1mP$	4 $\bar{3}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
48 $\bar{3}1mP$	4 $\bar{3}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
48 $\bar{3}1mP$	5 $\bar{3}12$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
48 $\bar{3}1mP$	5 $\bar{3}12$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
48 $\bar{3}1mP$	6 $\bar{3}1m$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
48 $\bar{3}1mP$	6 $\bar{3}1m$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{2 + 2c_1, 2 + 2c_1, 3 + 3c_1\}\}$	
48 $\bar{3}1mP$	6 $\bar{3}1m$	3 $\{(1, 0, 0), \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 3 + 3c_1\}\}$	
48 $\bar{3}1mP$	6 $\bar{3}1m$	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
48 $\bar{3}1mP$	7 $\bar{3}1m$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
48 $\bar{3}1mP$	7 $\bar{3}1m$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
49 $\bar{3}m1P$	2 $\bar{1}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
49 $\bar{3}m1P$	2 $\bar{1}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
49 $\bar{3}m1P$	2 $\bar{1}$	3 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 1\}\}$	
49 $\bar{3}m1P$	2 $\bar{1}$	4 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 2\}\}$	
49 $\bar{3}m1P$	3 3	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
49 $\bar{3}m1P$	3 3	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
49 $\bar{3}m1P$	4 $\bar{3}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
49 $\bar{3}m1P$	4 $\bar{3}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
49 $\bar{3}m1P$	5 $\bar{3}21$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1\}\}$	
49 $\bar{3}m1P$	5 $\bar{3}21$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
49 $\bar{3}m1P$	5 $\bar{3}21$	3 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 2\}\}$	
49 $\bar{3}m1P$	5 $\bar{3}21$	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
49 $\bar{3}m1P$	6 $\bar{3}m1$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
49 $\bar{3}m1P$	7 $\bar{3}m1$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
49 $\bar{3}m1P$	7 $\bar{3}m1$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
50 $\bar{3}mR$	2 $\bar{1}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
50 $\bar{3}mR$	2 $\bar{1}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{1, 1, 2\}\}$	
50 $\bar{3}mR$	2 $\bar{1}$	3 $\{(1, 0, 0), \{1, 2, 0\}, \{1, 0, 2\}\}$	
50 $\bar{3}mR$	2 $\bar{1}$	4 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 2\}\}$	
50 $\bar{3}mR$	3 3	1 $\{(1, 0, 0), \{0, 1, 0\}, \{c_1, c_1, 1 + c_1\}\}$	
50 $\bar{3}mR$	4 $\bar{3}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{1, 1, 2\}\}$	
50 $\bar{3}mR$	4 $\bar{3}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
50 $\bar{3}mR$	5 $\bar{3}21$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{1, 1, 2\}\}$	
50 $\bar{3}mR$	5 $\bar{3}21$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
50 $\bar{3}mR$	6 $\bar{3}m1$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{c_1, c_1, 1 + c_1\}\}$	
50 $\bar{3}mR$	7 $\bar{3}m1$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{1, 1, 2\}\}$	
50 $\bar{3}mR$	7 $\bar{3}m1$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
51 $\bar{6}P$	2 2_z	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
51 $\bar{6}P$	2 2_z	2 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
51 $\bar{6}P$	3 3	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
51 $\bar{6}P$	3 3	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
51 $\bar{6}P$	4 $\bar{6}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
52 $\bar{6}P$	2 m_z	1 $\{(1 + c_1, 0, 0), \{0, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
52 $\bar{6}P$	2 m_z	2 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + d_1), (1 + c_1)(2 + d_1 + d_2), 0\}, \{0, 0, 1\}\}$	6
52 $\bar{6}P$	2 m_z	3 $\{(1 + c_1, 0, 0), \{0, 1 + c_1, 0\}, \{0, 0, 2\}\}$	
52 $\bar{6}P$	2 m_z	4 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + d_1), (1 + c_1)(2 + d_1 + d_2), 0\}, \{0, 0, 2\}\}$	6
52 $\bar{6}P$	2 m_z	5 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + 2d_1), (1 + c_1)(3 + 2d_1 + d_2), 0\}, \{0, 1, 2\}\}$	29
52 $\bar{6}P$	2 m_z	6 $\{(1 + c_1, 0, 0), \{2(1 + c_1)(1 + d_1), 2(1 + c_1)(2 + d_1 + d_2), 0\}, \{1, 0, 2\}\}$	8
52 $\bar{6}P$	2 m_z	7 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + d_1), (1 + c_1)(4 + d_1 + 2d_2), 0\}, \{1, 1, 2\}\}$	36
52 $\bar{6}P$	3 3	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
52 $\bar{6}P$	3 3	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
52 $\bar{6}P$	4 $\bar{6}$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1\}\}$	
52 $\bar{6}P$	4 $\bar{6}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
52 $\bar{6}P$	4 $\bar{6}$	3 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 2\}\}$	
52 $\bar{6}P$	4 $\bar{6}$	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
53 $\bar{6}/mP$	2 $\bar{1}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
53 $\bar{6}/mP$	2 $\bar{1}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
53 $\bar{6}/mP$	2 $\bar{1}$	3 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 1\}\}$	
53 $\bar{6}/mP$	2 $\bar{1}$	4 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 2\}\}$	

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
53 $\bar{6}/mP$	3 2_z	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
53 $\bar{6}/mP$	3 2_z	2 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
53 $\bar{6}/mP$	4 m_z	1 $\{(1 + c_1, 0, 0), \{0, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
53 $\bar{6}/mP$	4 m_z	2 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + d_1), (1 + c_1)(2 + d_1 + d_2), 0\}, \{0, 0, 1\}\}$	6
53 $\bar{6}/mP$	4 m_z	3 $\{(1 + c_1, 0, 0), \{0, 1 + c_1, 0\}, \{0, 0, 2\}\}$	
53 $\bar{6}/mP$	4 m_z	4 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + d_1), (1 + c_1)(2 + d_1 + d_2), 0\}, \{0, 0, 2\}\}$	6
53 $\bar{6}/mP$	4 m_z	5 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + 2d_1), (1 + c_1)(3 + 2d_1 + d_2), 0\}, \{0, 1, 2\}\}$	29
53 $\bar{6}/mP$	4 m_z	6 $\{(1 + c_1, 0, 0), \{2(1 + c_1)(1 + d_1), 2(1 + c_1)(2 + d_1 + d_2), 0\}, \{1, 0, 2\}\}$	8
53 $\bar{6}/mP$	4 m_z	7 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + d_1), (1 + c_1)(4 + d_1 + 2d_2), 0\}, \{1, 1, 2\}\}$	36
53 $\bar{6}/mP$	5 $2/m_z$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
53 $\bar{6}/mP$	5 $2/m_z$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
53 $\bar{6}/mP$	5 $2/m_z$	3 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 1\}\}$	
53 $\bar{6}/mP$	5 $2/m_z$	4 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 2\}\}$	
53 $\bar{6}/mP$	6 $\bar{3}$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
53 $\bar{6}/mP$	6 $\bar{3}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
53 $\bar{6}/mP$	7 $\bar{3}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
53 $\bar{6}/mP$	7 $\bar{3}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
53 $\bar{6}/mP$	8 $\bar{6}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
53 $\bar{6}/mP$	9 $\bar{6}$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1\}\}$	
53 $\bar{6}/mP$	9 $\bar{6}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
53 $\bar{6}/mP$	9 $\bar{6}$	3 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 2\}\}$	
53 $\bar{6}/mP$	9 $\bar{6}$	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
53 $\bar{6}/mP$	10 $\bar{6}/m$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
53 $\bar{6}/mP$	10 $\bar{6}/m$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
54 $\bar{6}22P$	2 2_z	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
54 $\bar{6}22P$	2 2_z	2 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
54 $\bar{6}22P$	3 $\bar{3}$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
54 $\bar{6}22P$	3 $\bar{3}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
54 $\bar{6}22P$	4 $\bar{3}12$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
54 $\bar{6}22P$	4 $\bar{3}12$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
54 $\bar{6}22P$	5 $\bar{3}21$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1\}\}$	
54 $\bar{6}22P$	5 $\bar{3}21$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
54 $\bar{6}22P$	5 $\bar{3}21$	3 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 2\}\}$	
54 $\bar{6}22P$	5 $\bar{3}21$	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
54 $\bar{6}22P$	6 $\bar{6}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
54 $\bar{6}22P$	7 $\bar{6}22$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
54 $\bar{6}22P$	7 $\bar{6}22$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
55 $\bar{6}mmP$	2 2_z	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
55 $\bar{6}mmP$	2 2_z	2 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
55 $\bar{6}mmP$	3 $\bar{3}$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
55 $\bar{6}mmP$	3 $\bar{3}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
55 $\bar{6}mmP$	4 $\bar{3}m1$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
55 $\bar{6}mmP$	5 $\bar{3}1m$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
55 $\bar{6}mmP$	5 $\bar{3}1m$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
55 $\bar{6}mmP$	6 $\bar{6}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
55 $\bar{6}mmP$	7 $\bar{6}mm$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
56 $\bar{6}m2P$	2 m_z	1 $\{(1 + c_1, 0, 0), \{0, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
56 $\bar{6}m2P$	2 m_z	2 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + d_1), (1 + c_1)(2 + d_1 + d_2), 0\}, \{0, 0, 1\}\}$	32
56 $\bar{6}m2P$	2 m_z	3 $\{(1 + c_1, 0, 0), \{0, 1 + c_1, 0\}, \{0, 0, 2\}\}$	
56 $\bar{6}m2P$	2 m_z	4 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + d_1), (1 + c_1)(2 + d_1 + d_2), 0\}, \{0, 0, 2\}\}$	32
56 $\bar{6}m2P$	2 m_z	5 $\{(1 + c_1, 0, 0), \{2(1 + c_1)(1 + d_1), 2(1 + c_1)(2 + d_1 + d_2), 0\}, \{1, 0, 2\}\}$	30
56 $\bar{6}m2P$	3 $\bar{3}$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
56 $\bar{6}m2P$	3 $\bar{3}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
56 $\bar{6}m2P$	4 $\bar{3}12$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
56 $\bar{6}m2P$	4 $\bar{3}12$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
56 $\bar{6}m2P$	5 $\bar{3}m1$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
56 $\bar{6}m2P$	6 $\bar{6}$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1\}\}$	
56 $\bar{6}m2P$	6 $\bar{6}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
56 $\bar{6}m2P$	6 $\bar{6}$	3 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 2\}\}$	
56 $\bar{6}m2P$	6 $\bar{6}$	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
56 $\bar{6}m2P$	7 $\bar{6}m2$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
56 $\bar{6}m2P$	7 $\bar{6}m2$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
57 $\bar{6}2mP$	2 m_z	1 $\{(1 + c_1, 0, 0), \{0, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
57 $\bar{6}2mP$	2 m_z	2 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + d_1), (1 + c_1)(2 + d_1 + d_2), 0\}, \{0, 0, 1\}\}$	
57 $\bar{6}2mP$	2 m_z	3 $\{(1 + c_1, 0, 0), \{0, 1 + c_1, 0\}, \{0, 0, 2\}\}$	32
57 $\bar{6}2mP$	2 m_z	4 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + d_1), (1 + c_1)(2 + d_1 + d_2), 0\}, \{0, 0, 2\}\}$	
57 $\bar{6}2mP$	2 m_z	5 $\{(1 + c_1, 0, 0), \{2(1 + c_1)(1 + d_1), 2(1 + c_1)(2 + d_1 + d_2), 0\}, \{1, 0, 2\}\}$	32
57 $\bar{6}2mP$	3 $\bar{3}$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	30
57 $\bar{6}2mP$	3 $\bar{3}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
57 $\bar{6}2mP$	4 $\bar{3}21$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1\}\}$	
57 $\bar{6}2mP$	4 $\bar{3}21$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
57 $\bar{6}2mP$	4 $\bar{3}21$	3 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 2\}\}$	
57 $\bar{6}2mP$	4 $\bar{3}21$	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
57 $\bar{6}2mP$	5 $\bar{3}1m$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
57 $\bar{6}2mP$	5 $\bar{3}1m$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
57 $\bar{6}2mP$	6 $\bar{6}$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1\}\}$	
57 $\bar{6}2mP$	6 $\bar{6}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	

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Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
57 $\bar{6}2mP$	6 $\bar{6}$	3 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 2\}\}$	
57 $\bar{6}2mP$	6 $\bar{6}$	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
57 $\bar{6}2mP$	7 $\bar{6}2m$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1\}\}$	
57 $\bar{6}2mP$	7 $\bar{6}2m$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
57 $\bar{6}2mP$	7 $\bar{6}2m$	3 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 2\}\}$	
57 $\bar{6}2mP$	7 $\bar{6}2m$	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	2 $\bar{1}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	2 $\bar{1}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	2 $\bar{1}$	3 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	2 $\bar{1}$	4 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	3 2_z	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
58 $6/mmmP$	3 2_z	2 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
58 $6/mmmP$	4 m_z	1 $\{(1 + c_1, 0, 0), \{0, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	4 m_z	2 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + d_1), (1 + c_1)(2 + d_1 + d_2), 0\}, \{0, 0, 1\}\}$	32
58 $6/mmmP$	4 m_z	3 $\{(1 + c_1, 0, 0), \{0, 1 + c_1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	4 m_z	4 $\{(1 + c_1, 0, 0), \{(1 + c_1)(1 + d_1), (1 + c_1)(2 + d_1 + d_2), 0\}, \{0, 0, 2\}\}$	32
58 $6/mmmP$	4 m_z	5 $\{(1 + c_1, 0, 0), \{2(1 + c_1)(1 + d_1), 2(1 + c_1)(2 + d_1 + d_2), 0\}, \{1, 0, 2\}\}$	30
58 $6/mmmP$	5 $2/m_z$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	5 $2/m_z$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	5 $2/m_z$	3 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	5 $2/m_z$	4 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	6 3	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
58 $6/mmmP$	6 3	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
58 $6/mmmP$	7 $\bar{3}$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	7 $\bar{3}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	8 312	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	8 312	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	9 321	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	9 321	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	9 321	3 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	9 321	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	10 $3m1$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
58 $6/mmmP$	11 $31m$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1 + c_1\}\}$	
58 $6/mmmP$	11 $31m$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
58 $6/mmmP$	12 $\bar{3}1m$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	12 $\bar{3}1m$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	13 $\bar{3}m1$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	13 $\bar{3}m1$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	14 6	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
58 $6/mmmP$	15 $\bar{6}$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	15 $\bar{6}$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	15 $\bar{6}$	3 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	15 $\bar{6}$	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	16 $6/m$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	16 $6/m$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	17 622	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	17 622	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	18 $6mm$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
58 $6/mmmP$	19 $\bar{6}m2$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	19 $\bar{6}m2$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	20 $\bar{6}2m$	1 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	20 $\bar{6}2m$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	20 $\bar{6}2m$	3 $\{(1, 0, 0), \{2, 3, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	20 $\bar{6}2m$	4 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
58 $6/mmmP$	21 $6/mmm$	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
58 $6/mmmP$	21 $6/mmm$	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 2\}\}$	
59 $23P$	2 222	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
59 $23P$	2 222	2 $\{(1, 0, 0), \{0, 1, 0\}, \{1, 1, 2\}\}$	
59 $23P$	2 222	3 $\{(1, 0, 0), \{1, 2, 0\}, \{1, 0, 2\}\}$	
59 $23P$	2 222	4 $\{(2, 0, 0), \{0, 2, 0\}, \{0, 0, 2\}\}$	
59 $23P$	3 23	1 $\{(1, 0, 0), \{0, 1, 0\}, \{1, 1, 2\}\}$	
59 $23P$	3 23	2 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
60 $23F$	2 222	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
60 $23F$	2 222	2 $\{(1, 0, 0), \{1, 2, 0\}, \{1, 0, 2\}\}$	
60 $23F$	3 23	1 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
61 $23I$	2 222	1 $\{(1, 0, 0), \{0, 1, 0\}, \{3, 3, 4\}\}$	
61 $23I$	2 222	2 $\{(1, 0, 0), \{0, 1, 0\}, \{1, 1, 2\}\}$	
61 $23I$	2 222	3 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
61 $23I$	2 222	4 $\{(1, 0, 0), \{0, 1, 0\}, \{3, 3, 4\}\}$	
61 $23I$	2 222	5 $\{(1, 0, 0), \{0, 1, 0\}, \{1, 1, 2\}\}$	
61 $23I$	2 222	6 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
61 $23I$	3 23	1 $\{(1, 0, 0), \{0, 1, 0\}, \{3, 3, 4\}\}$	
61 $23I$	3 23	2 $\{(1, 0, 0), \{0, 1, 0\}, \{1, 1, 2\}\}$	
61 $23I$	3 23	3 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	
61 $23I$	3 23	4 $\{(1, 0, 0), \{0, 1, 0\}, \{3, 3, 4\}\}$	
61 $23I$	3 23	5 $\{(1, 0, 0), \{0, 1, 0\}, \{1, 1, 2\}\}$	
61 $23I$	3 23	6 $\{(1, 0, 0), \{0, 1, 0\}, \{0, 0, 1\}\}$	

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
62 $m\bar{3}P$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
62 $m\bar{3}P$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
62 $m\bar{3}P$	2 $\bar{1}$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
62 $m\bar{3}P$	2 $\bar{1}$	4 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
62 $m\bar{3}P$	3 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
62 $m\bar{3}P$	3 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
62 $m\bar{3}P$	3 222	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
62 $m\bar{3}P$	3 222	4 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
62 $m\bar{3}P$	4 mmm	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
62 $m\bar{3}P$	4 mmm	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
62 $m\bar{3}P$	4 mmm	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
62 $m\bar{3}P$	4 mmm	4 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
62 $m\bar{3}P$	5 23	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
62 $m\bar{3}P$	5 23	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
62 $m\bar{3}P$	6 $m\bar{3}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
62 $m\bar{3}P$	6 $m\bar{3}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
63 $m\bar{3}F$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
63 $m\bar{3}F$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
63 $m\bar{3}F$	2 $\bar{1}$	3 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
63 $m\bar{3}F$	3 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
63 $m\bar{3}F$	3 222	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
63 $m\bar{3}F$	4 mmm	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
63 $m\bar{3}F$	4 mmm	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
63 $m\bar{3}F$	5 23	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
63 $m\bar{3}F$	6 $m\bar{3}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
64 $m\bar{3}I$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
64 $m\bar{3}I$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
64 $m\bar{3}I$	2 $\bar{1}$	3 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
64 $m\bar{3}I$	3 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
64 $m\bar{3}I$	3 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
64 $m\bar{3}I$	3 222	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
64 $m\bar{3}I$	3 222	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
64 $m\bar{3}I$	3 222	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
64 $m\bar{3}I$	3 222	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
64 $m\bar{3}I$	4 mmm	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
64 $m\bar{3}I$	4 mmm	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
64 $m\bar{3}I$	5 23	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
64 $m\bar{3}I$	5 23	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
64 $m\bar{3}I$	5 23	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
64 $m\bar{3}I$	5 23	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
64 $m\bar{3}I$	5 23	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
64 $m\bar{3}I$	5 23	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
64 $m\bar{3}I$	6 $m\bar{3}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
64 $m\bar{3}I$	6 $m\bar{3}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
65 432P	2 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
65 432P	2 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
65 432P	2 222	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
65 432P	2 222	4 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
65 432P	3 23	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
65 432P	3 23	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
65 432P	4 432	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
65 432P	4 432	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
66 432F	2 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
66 432F	2 222	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
66 432F	3 23	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
66 432F	4 432	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
67 432I	2 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
67 432I	2 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
67 432I	2 222	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
67 432I	2 222	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
67 432I	2 222	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
67 432I	2 222	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
67 432I	3 23	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
67 432I	3 23	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
67 432I	3 23	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
67 432I	3 23	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
67 432I	3 23	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
67 432I	3 23	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
67 432I	4 432	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
67 432I	4 432	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
68 43mP	2 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
68 43mP	2 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
68 43mP	2 222	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
68 43mP	2 222	4 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
68 43mP	3 23	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
68 43mP	3 23	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
68 43mP	4 43m	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
68 $4\bar{3}mP$	4 $4\bar{3}m$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
69 $4\bar{3}mF$	2 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
69 $4\bar{3}mF$	2 222	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
69 $4\bar{3}mF$	3 23	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
69 $4\bar{3}mF$	4 $4\bar{3}m$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
70 $4\bar{3}mI$	2 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
70 $4\bar{3}mI$	2 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
70 $4\bar{3}mI$	2 222	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
70 $4\bar{3}mI$	2 222	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
70 $4\bar{3}mI$	2 222	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
70 $4\bar{3}mI$	2 222	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
70 $4\bar{3}mI$	3 23	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
70 $4\bar{3}mI$	3 23	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
70 $4\bar{3}mI$	3 23	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
70 $4\bar{3}mI$	3 23	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
70 $4\bar{3}mI$	3 23	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
70 $4\bar{3}mI$	3 23	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
70 $4\bar{3}mI$	4 $4\bar{3}m$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
70 $4\bar{3}mI$	4 $4\bar{3}m$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
70 $4\bar{3}mI$	4 $4\bar{3}m$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
70 $4\bar{3}mI$	4 $4\bar{3}m$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
70 $4\bar{3}mI$	4 $4\bar{3}m$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
70 $4\bar{3}mI$	4 $4\bar{3}m$	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
71 $m\bar{3}mP$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
71 $m\bar{3}mP$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
71 $m\bar{3}mP$	2 $\bar{1}$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
71 $m\bar{3}mP$	2 $\bar{1}$	4 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
71 $m\bar{3}mP$	3 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
71 $m\bar{3}mP$	3 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
71 $m\bar{3}mP$	3 222	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
71 $m\bar{3}mP$	3 222	4 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
71 $m\bar{3}mP$	4 mmm	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
71 $m\bar{3}mP$	4 mmm	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
71 $m\bar{3}mP$	4 mmm	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
71 $m\bar{3}mP$	4 mmm	4 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
71 $m\bar{3}mP$	5 23	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
71 $m\bar{3}mP$	5 23	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
71 $m\bar{3}mP$	6 $m\bar{3}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
71 $m\bar{3}mP$	6 $m\bar{3}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
71 $m\bar{3}mP$	7 432	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
71 $m\bar{3}mP$	7 432	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
71 $m\bar{3}mP$	8 $4\bar{3}m$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
71 $m\bar{3}mP$	8 $4\bar{3}m$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
71 $m\bar{3}mP$	9 $m\bar{3}m$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
71 $m\bar{3}mP$	9 $m\bar{3}m$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
72 $m\bar{3}mF$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
72 $m\bar{3}mF$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
72 $m\bar{3}mF$	2 $\bar{1}$	3 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
72 $m\bar{3}mF$	3 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
72 $m\bar{3}mF$	3 222	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
72 $m\bar{3}mF$	4 mmm	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
72 $m\bar{3}mF$	4 mmm	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
72 $m\bar{3}mF$	5 23	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
72 $m\bar{3}mF$	6 $m\bar{3}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
72 $m\bar{3}mF$	7 432	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
72 $m\bar{3}mF$	8 $4\bar{3}m$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
72 $m\bar{3}mF$	9 $m\bar{3}m$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
73 $m\bar{3}mI$	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
73 $m\bar{3}mI$	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
73 $m\bar{3}mI$	2 $\bar{1}$	3 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
73 $m\bar{3}mI$	3 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
73 $m\bar{3}mI$	3 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
73 $m\bar{3}mI$	3 222	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
73 $m\bar{3}mI$	3 222	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
73 $m\bar{3}mI$	3 222	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
73 $m\bar{3}mI$	3 222	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
73 $m\bar{3}mI$	4 mmm	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
73 $m\bar{3}mI$	4 mmm	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
73 $m\bar{3}mI$	5 23	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
73 $m\bar{3}mI$	5 23	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
73 $m\bar{3}mI$	5 23	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
73 $m\bar{3}mI$	5 23	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
73 $m\bar{3}mI$	5 23	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
73 $m\bar{3}mI$	5 23	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
73 $m\bar{3}mI$	6 $m\bar{3}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
73 $m\bar{3}mI$	6 $m\bar{3}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
73 $m\bar{3}mI$	7 432	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	

Continued on next page

Table S1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
73 $m\bar{3}mI$	7 432	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
73 $m\bar{3}mI$	8 $\bar{4}3m$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
73 $m\bar{3}mI$	8 $\bar{4}3m$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
73 $m\bar{3}mI$	8 $\bar{4}3m$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
73 $m\bar{3}mI$	8 $\bar{4}3m$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
73 $m\bar{3}mI$	8 $\bar{4}3m$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
73 $m\bar{3}mI$	8 $\bar{4}3m$	6 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
73 $m\bar{3}mI$	9 $m\bar{3}m$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
73 $m\bar{3}mI$	9 $m\bar{3}m$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	

Table S2: A list of extra d -variable conditions referenced in table S1. For each case number (c#) in the table, all variables are restricted to non-negative integer values, except for entries 39-42 where they are instead constrained by the inequalities presented and where d_1 can be negative. The cases are presented in a semi-arbitrary order determined using Mathematica's built-in Sort command.

c#	extra conditions
1	$\frac{5+4d_1+d_1^2}{4+2d_1}$
2	$\frac{2d_1(1+d_1)}{1+d_1+d_2}$
3	$\frac{1+2d_1+2d_1^2}{1+d_1+d_2}$
4	$\frac{2d_1(1+d_1)}{2+d_1+d_2}$
5	$\frac{d_1(2+d_1)}{2+d_1+d_2}$
6	$\frac{1+d_1+d_1^2}{2+d_1+d_2}$
7	$\frac{2+2d_1+d_1^2}{2+d_1+d_2}$
8	$\frac{3+6d_1+4d_1^2}{2(2+d_1+d_2)}$
9	$\frac{2d_1(1+d_1)}{3+d_1+d_2}$
10	$\frac{d_1(2+d_1)}{3+d_1+d_2}$
11	$\frac{3+d_1+d_2}{2+2d_1+d_1^2}$
12	$\frac{3+d_1+d_2}{2(2+3d_1+d_1^2)}$
13	$\frac{3+4d_1+d_1^2}{3+d_1+d_2}$
14	$\frac{5+4d_1+d_1^2}{3+d_1+d_2}$
15	$\frac{2(6+5d_1+d_1^2)}{3+d_1+d_2}$
16	$\frac{d_1(2+d_1)}{4+d_1+d_2}$
17	$\frac{2(2+3d_1+d_1^2)}{4+d_1+d_2}$
18	$\frac{3+4d_1+d_1^2}{4+d_1+d_2}$
19	$\frac{2(6+5d_1+d_1^2)}{4+d_1+d_2}$
20	$\frac{d_1(2+d_1)}{5+d_1+d_2}$
21	$\frac{3+4d_1+d_1^2}{5+d_1+d_2}$
22	$\frac{8+6d_1+d_1^2}{5+d_1+d_2}$
23	$\frac{1+2d_1+2d_1^2}{2+2d_1+d_2}$
24	$\frac{2d_1(1+d_1)}{3+2d_1+d_2}$
25	$\frac{3+8d_1+4d_1^2}{3+2d_1+d_2}$
26	$\frac{2(2+3d_1+d_1^2)}{4+2d_1+d_2}$
27	$\frac{5+2d_1+d_2}{4d_1(1+d_1)}$
28	$\frac{3+2d_1+2d_2}{1+2d_1+4d_1^2}$
29	$\frac{6+4d_1+2d_2}{2d_1(1+d_1)}$
30	$\frac{2d_1(1+d_1)}{2+d_1+d_2}$
31	$\frac{d_1(2+d_1)}{2+d_1+d_2}$
32	$\frac{1-d_1^2}{2+d_1+d_2}$
33	$\frac{d_1(2+d_1)}{3+d_1+d_2}$
34	$\frac{3+4d_1+d_1^2}{3+d_1+d_2}$
35	$\frac{1+d_1^2}{3+d_1+2d_2}$
36	$\frac{1+d_1+d_1^2}{4+d_1+2d_2}$
	$\frac{3+6d_1+4d_1^2}{2(2+d_1+d_2)}$
	$\frac{2+2d_1+d_1^2}{2+d_1+d_2}$
	$\frac{1+d_1+d_1^2}{2+2d_1+d_2}$
	$\frac{2+2d_1+d_1^2}{3+d_1+d_2}$
	$\frac{5+4d_1+d_1^2}{3+d_1+d_2}$
	$\frac{1+d_2+d_1(2+d_2)}{3+d_1+2d_2}$
	$\frac{3+2d_2+2d_1(2+d_2)}{2(4+d_1+2d_2)}$

Continued on next page

Table S2 – continued from previous page

c#	extra conditions		
37	$\frac{3+d_1}{6+2d_1+3d_2}$	$\frac{3+d_1}{3+d_1+d_2}$	
38	$\frac{1-d_1^2}{1+d_1+2d_2}$	$\frac{(1-d_1)d_2}{1+d_1+2d_2}$	$\frac{(1+d_1)(1+d_2)}{1+d_1+2d_2}$
39	$\frac{d_1(5+2d_1+3d_2)}{4+d_1+2d_2}$	$d_2 \geq \text{Max}[\frac{-1-2d_1}{2}, 0]$	d_1 can be negative
40	$\frac{d_1(7+2d_1+3d_2)}{4+d_1+2d_2}$	$d_2 \geq \text{Max}[\frac{-1-2d_1}{2}, 0]$	d_1 can be negative
41	$\frac{(1+d_1)(4+2d_1+3d_2)}{3+d_1+2d_2}$	$d_2 \geq \text{Max}[-d_1, 0]$	d_1 can be negative
42	$\frac{2d_1^2-d_2+d_1(2+3d_2)}{3+d_1+2d_2}$	$d_2 \geq \text{Max}[-d_1, 0]$	d_1 can be negative
43	$\frac{2(2+d_1)d_2(1+d_2)}{3+d_1+2d_2+d_1d_2+d_3}$	$\frac{2(3+d_1+2d_2+d_1d_2+d_3)}{2+d_1}$	
44	$\frac{(1+d_1)(3+8d_2+4d_2^2)}{4+2d_2+d_1(3+2d_2)+d_3}$	$\frac{4+3d_1+2d_2+2d_1d_2+d_3}{1+d_1}$	
45	$\frac{2(1+d_1)(1+d_3)}{7+4d_3+d_2(2+d_3)+d_1(3+2d_3)}$	$\frac{4+2d_1+d_2}{2(2+d_1)}$	
46	$\frac{8+5d_3+d_2(2+d_3)+d_1(3+2d_3)}{2(3+d_1)(1+d_3)}$	$\frac{5+2d_1+d_2}{2(3+d_1)}$	
47	$\frac{9+6d_3+d_2(2+d_3)+d_1(3+2d_3)}{(1+d_1)(1+2d_3)}$	$\frac{6+2d_1+d_2}{1+d_1}$	
48	$\frac{5+4d_3+2d_1(1+d_3)+d_2(3+2d_3)}{(2+d_1)(1+2d_3)}$	$\frac{2+d_1+d_2}{2+d_1}$	
49	$\frac{7+6d_3+2d_1(1+d_3)+d_2(3+2d_3)}{(3+d_1)(3+2d_3)}$	$\frac{3+d_1+d_2}{3+d_1}$	
50	$\frac{6(2+d_3)+2d_1(2+d_3)+d_2(5+2d_3)}{3+d_1+d_2}$	$\frac{3+d_1+d_2}{3+d_1+d_2}$	

2 Algorithm details

As stated in the body text of the article, the essential challenge with each of the many processing steps that we applied to the Mathematica’s Reduce output was to modify the symbolic form of B_N and its conditions without altering the solution space that they represent (i.e. the space of normally supportive sublattices). Thus every step of the processing yields a correct form but not necessarily a form that looks nice or is easy to understand. This effort required considerable attention to detail. Depending on the specific case, the output from Reduce can take on a variety of different forms. A major component of the present research effort was devoted to bringing the output to a uniform format that follows relatively nice rules. First, simple steps were taken to extract information about the B_N matrix and the conditions on its elements, eliminate special conditions that were obviously true, simplify complicated logical statements, and separate joint statements into lists of simultaneous conditions. A number of subroutines were then developed in order to further shape the output, each one handling a specific issue. Each paragraph below describes the function of one of these subroutines. The Mathematica code used to perform these calculations is also provided in a separate file.

To make each triplet look uniform, each variable is presented in the form of a letter combined with a number. Each variable that appears in an extra condition is denoted as d_n while all the other variables are denoted as c_n where n is an integer. Each variable is then numbered in the order that it appears in the B_N matrix, starting from the top and left side and proceeding row by row with the c variables and d variables numbered separately (i.e. a triplet can contain both c_1 and d_1). Because many of the subroutines introduce new variables into the triplets they modify, it was convenient to periodically relabel all of the variables in a triplet in a uniform way during the multi-step reduction process.

The extra conditions often took the form of an integer divided by a lone variable. To simplify this, we set the variable to a divisor of the numerator. Doing this can have multiple solutions when the numerator has multiple divisors. In such a case, the triplet bifurcates into multiple less complicated triplets, one for each solution.

The Reduce command sometimes leaves residual quotients in the B_N matrix. Since each B_N must be in Hermite normal form, its entries must all be integers. For this reason, it was convenient to replace such a quotient with a new variable in B_N , and then solve for one of the other variables, adding the resulting quotient to the list of extra conditions in the last portion of the triplet.

Most of these subroutines aim to simplify the extra conditions, which sometimes leaves extra conditions that are unnecessary, redundant, or sometimes even impossible to satisfy. In the event that a triplet contains an extra condition that cannot possibly be an integer, such as $d_2 + \frac{1}{2}$, it does not represent any possible normally supportive sublattices, and thus the entire triplet can be deleted. In the event that an extra condition is obviously an integer, e.g. 2 , $d_1 + 1$, $2d_2(1 - d_2)$, etc., we needn't keep track of it and thus it can be removed from the list of extra conditions. In the event that two extra conditions are linearly dependent, for example $\frac{1-d_3^2}{2}$ and $\frac{1-d_3^2}{2d_2}$, the less restricting of the two ($\frac{1-d_3^2}{2}$ in our example) is redundant and can be removed from the list of extra conditions. This subroutine is implemented frequently because many of the other subroutines change the extra conditions so as to produce triplets that need cleaning.

After removing the quotients from the B_N matrices, some quotients are introduced into the conditions. This often tends to make the ranges on variables very complicated. To remedy this, we again use the Reduce command, but this time only on the obviously complicated conditions. This step sometimes has the side effect of making a single triplet split into multiple but nicer looking triplets.

In some cases, there are extra conditions in the form $\frac{n_1}{n_2}d$ where d is a variable in the B_N matrix and n_1 and n_2 are coprime integers. These cases can be simplified a little because the only values of d that will satisfy this condition are multiples of n_2 . We simply let $h = d/n_2$, and then replace all instances of d in the triplet with n_2h so that we end up with one less extra condition in these cases (the h will then be relabeled as a new c or d variable).

Sometimes there are extra conditions wherein a variable appears only once in the numerator of an extra condition. In other words, the extra condition has the form $\frac{polynomial_1 + nd}{polynomial_2}$ where n is a constant integer, d is a variable in the B_N matrix and the *polynomials* do not contain the variable d . This condition can be eliminated with a little work. If we let $\frac{polynomial_1 + nd}{polynomial_2} = k$ then we can replace all instances of d in the triplet with $\frac{1}{n}(kpolynomial_2 - polynomial_1)$ which will eliminate this extra condition (k will then be relabeled as a new c or d variable). The standard form doesn't allow any variable expression in B_N that are not obviously integers. To avoid introducing numerical fractions in B_N in this step, we make a second replacement to remove any $\frac{1}{n}$ that might appear in the triplet.

Sometimes the output of Reduce has more variables than is necessary. For example, a particular B_N matrix might have only three elements with variables which have the form $2(3 + d_1 + d_2 + d_3)$, $2(4 + d_1 + 2d_2)$, and $4(3 + d_1 + d_2 + d_3)$. By inspection it can be seen that the third element is exactly double the first element and thus there are only two linearly independent polynomials. This is a problem because there are three variables to span B_N which means that there are redundancies. The desired format is by definition free of variable redundancies – it doesn't permit more than one set of variable values to achieve the same numerical B_N matrix. To fix this problem, it was necessary to rewrite these polynomials in terms of only two variables that span the same B_N space. To do this we implemented Mathematica's GroebnerBasis command which takes a series of polynomials and returns a set of linearly independent polynomials that span the same space. In the example above, the Gröbner basis is $\{d_2 - d_3, d_1 + 2d_3\}$. If we let $f_1 = d_2 - d_3$ and $f_2 = d_1 + 2d_3$ then we can replace every instance of d_1 with $f_2 - 2d_3$ and every instance of d_2 with $f_1 + d_3$ then the original expressions above become $2(3 + f_1 + f_2)$, $2(1 + 2f_1 + f_2)$, and $4(3 + f_1 + f_2)$ which has only two variables; the f variables will then be relabeled as c or d variables.

While the subroutine described in the previous paragraph does an excellent job at removing unnecessary variables in the B_N matrices, it fails to reduce the corresponding number of variables in the list of conditions. To illustrate this problem, consider the example in the previous paragraph where d_1 , d_2 , and d_3 could be any non-negative integer. After replacing d_1 with $f_2 - 2d_3$ and d_2 with $f_1 + d_3$, our conditions become $f_2 - 2d_3 \geq 0$, $f_1 + d_3 \geq 0$, and $d_3 \geq 0$. It is no longer necessary to keep track of d_3 since it was eliminated from B_N . To eliminate d_3 from the conditions, we first isolate it in each inequality which $f_2/2 \geq d_3$, $d_3 \geq -f_1$, and $d_3 \geq 0$. We can then combine these three conditions into the following two compound inequalities $f_2/2 \geq d_3 \geq 0$ and $f_2/2 \geq d_3 \geq -f_1$. Since the value of d_3 makes no difference in B_N , we can choose to set it equal to the shared maximum

value in both compound inequalities which then simplifies them to $f_2/2 \geq 0$ and $f_2/2 \geq -f_1$ and thus d_3 is now completely removed from the triplet. This subroutine has the unfortunate side effect of leaving somewhat awkward conditions, which are later improved by the subroutine that reapplies Reduce to the conditions as described above.

The order in which the subroutines were applied is somewhat strategic and somewhat arbitrary. Often, the application of one subroutine recreated undesirable structures within the matrix or conditions that were resolved by a previous subroutine, so that the first subroutine needed to be reapplied. This led to seemingly arbitrary iterations in the application of certain groups of subroutines. The specific and rather delicate ordering of subroutine calls that we ultimately converged on did bring all cases into the desired uniform format; but it is likely that other orderings might also accomplish this. We also point out that seemingly minor deviations from our final processing-step order sometimes fail spectacularly to deliver the desired format.