

!Atom name	number	x	y	z	Biso	Occ
Atom Li1+	4	2/3	1/3	-0.167	0.8	1.0
		0.00	0.00	1.00	1.00	0.00

Layer 2 = 1

Layer 3 = 1

Stacking

!stacking type

Recursive

!number of layers

infinite

Transitions

!layer 1 to layer 1

LT	0.00000000	0.000000	0.000000	1/3		
	0.000000	0.000000	0.000000	0.000000		
FW	0.00	0.00	0.00	0.00	0.00	0.00
	0.00	0.00	0.00	0.00	0.00	0.00

!layer 1 to layer 2

LT	1.00	2/3	1/3	1/3		
	21.000000	0.000000	0.000000	0.000000		
FW	0.00	0.00	0.00	0.00	0.00	0.00
	0.00	0.00	0.00	0.00	0.00	0.00

!layer 1 to layer 3

LT	0.000000	0.000000	0.000000	0.000000		
	0.000000	0.000000	0.000000	0.000000		
FW	0.00	0.00	0.00	0.00	0.00	0.00
	0.00	0.00	0.00	0.00	0.00	0.00

!layer 2 to layer 1

LT	0.000000	0.000000	0.000000	0.000000		
	0.000000	0.000000	0.000000	0.000000		
FW	0.00	0.00	0.00	0.00	0.00	0.00
	0.00	0.00	0.00	0.00	0.00	0.00

!layer 2 to layer 2

LT	0.000000	0.000000	0.000000	0.0000		
	0.000000	0.000000	0.000000	0.000000		
FW	0.00	0.00	0.00	0.00	0.00	0.00
	0.00	0.00	0.00	0.00	0.00	0.00

!layer 2 to layer 3

LT	1.00	2/3	1/3	1/3		
	31.000000	0.000000	0.000000	0.000000		
FW	0.00	0.00	0.00	0.00	0.00	0.00
	0.00	0.00	0.00	0.00	0.00	0.00

!layer 3 to layer 1