

Apr 08, 15 16:43		Li2TeC2-P-3m1-DFT-ent.txt										Page 1/1	
HEADER	generated from xyz												
CRYST1	4.3556	4.3533	6.0533	89.89	90.01	120.02	P1						
SCALE1	0.229593	0.132654	-0.000131	0.000000									
SCALE2	0.000004	0.265301	-0.000284	0.000000									
SCALE3	0.000008	-0.000188	0.165198	0.000000									
HETATM	1	Te1	UNK	1	0.000	0.000	0.000	1.00	0.00	Te			
HETATM	2	Li1	UNK	1	2.178	1.262	4.450	1.00	0.00	Li			
HETATM	3	C1	UNK	1	0.000	0.003	3.659	1.00	0.00	C			
HETATM	4	C1	UNK	1	0.000	0.003	2.395	1.00	0.00	C			
HETATM	5	Li1	UNK	1	0.000	2.514	1.607	1.00	0.00	Li			
MASTER	0	0	0	0	0	0	0	3	2	0	2	0	
END													