

Apr 08, 15 16:48		Na <sub>2</sub> TeC <sub>2</sub> -I4mmm-DFT-ent.txt										Page 1/1	
HEADER	generated from xyz												
CRYST1	5.7340	5.7340	6.1357	90.00	90.00	90.00	P1						
SCALE1	0.174398	-0.000000	0.000000	0.000000									
SCALE2	-0.000000	0.174398	0.000000	0.000000									
SCALE3	0.000000	0.000000	0.162981	0.000000									
HETATM	1	C1	UNK	1	0.000	0.000	5.505	1.00	0.00	C			
HETATM	2	Na1	UNK	1	0.000	2.867	1.534	1.00	0.00	Na			
HETATM	3	Te1	UNK	1	0.000	0.000	3.068	1.00	0.00	Te			
HETATM	4	C1	UNK	1	0.000	0.000	0.631	1.00	0.00	C			
HETATM	5	Na1	UNK	1	2.867	0.000	4.602	1.00	0.00	Na			
HETATM	6	C1	UNK	1	2.867	2.867	2.437	1.00	0.00	C			
HETATM	7	C1	UNK	1	2.867	2.867	3.699	1.00	0.00	C			
HETATM	8	Na1	UNK	1	0.000	2.867	4.602	1.00	0.00	Na			
HETATM	9	Na1	UNK	1	2.867	0.000	1.534	1.00	0.00	Na			
HETATM	10	Te1	UNK	1	2.867	2.867	0.000	1.00	0.00	Te			
MASTER	0	0	0	0	0	0	0	3	2	0	2	0	
END													