1 .__ . . . () **223**, 369 (2001)

 $_ _^{\land} _^{\land} = 1.50.A$; 63.20.; 64.60.



 $\begin{array}{c} \bullet & \bullet \\ \bullet & \bullet$ $I_{\pm}ab?$ $e_{\pm} = e\beta - S_{\pm} \cdot c \cdot e = \Gamma$ 10 _____ 10 2 (a) TA(X) phonon in Na@i structure Ψ - ΨΨ 1 β-Ψ_ 1.Ψ ...Ψ 1 3

 $\mathbf{v} \quad \begin{bmatrix} 00\xi \end{bmatrix}_{\wedge} \mathbf{W} \quad \mathbf{v} \quad \mathbf{W}, \quad \boldsymbol{\xi} \approx 0.5 \quad \mathbf{v}$ $\begin{bmatrix} 100g \\ - & 1 \end{bmatrix} \begin{bmatrix} - & 1 \end{bmatrix} \begin{bmatrix} - & 1 \end{bmatrix} \begin{bmatrix} - & 0 \end{bmatrix} \begin{bmatrix} - & 0$ 5 $\begin{array}{c} A(\) & & A(\$

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|-------------------|---|--|---|--------------|------------|
| | v | _^ | _^ ¥ ¶ _(^ ¥ 1) | | ¥ |
| (1) | ₩ > > (⁷ / ₄) | $(1,1,0), (\bar{1},1,0),$ | $ \begin{array}{c} - & = & A_1(\begin{array}{c} - \\ 2 \end{array}) \\ (0, 0, 1) \ \underline{} 2 \end{array} ; 2 \ (439) \end{array} $ | 4 (10) |) ≞,_^ , , |
| (2) (3) | $-\frac{4}{43}$ $(\frac{18}{4})$ | (0,0,2), (2,0,0), (2,0,0), (2,0,0), (0,2,0), (| (0,2,0) &; 8 (471) (0,0,2) ,2; 6; 8 (653) | _ 16 _ 16 | ▼ ' 4 3 |
| (4) (5) (6) | $\begin{array}{c} -\underline{\wedge} & (\begin{array}{c} 26\\ 2 \end{array}) \\ -\underline{42} & (\begin{array}{c} 11\\ 2 \end{array}) \\ 222(\begin{array}{c} 8 \end{array}) \end{array}$ | (0,0,2), (2,0,0), (0,0,2), (2,0,0), (| (0,2,0) A ; 4; 8 (317) (0,2,0) $2; 2; 4; 8 (417)(0,0,2)$ $2; 2; 2; 4; 8 (417)$ | 16 16 | |
| (1) | -222(2) | (2,0,0), (0,2,0), $(1,0,\bar{1}), (0,1,0).$ | $(0, 0, 2) \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$ | .05) _ 10 | |