Anharmonic properties of the vibrational quantum computer

Chemistry Department, Wehr Chemistry Building, Marquette University, Milwaukee, Wisconsin 53201-1881

(R[illegible] 29 J[illegible] 2007; [illegible] 10 A[illegible] 2007; [illegible] 24 M[illegible] 2007)

[illegible]

II. THEORY

A [illegible]

$$M_{kl,ij} = \square_0 \square k \square i \square_{Q_1} \square l \square j \square_{Q_2} + \square_1 \square k \square Q_1 \square i \square_{Q_1} \square l \square$$

. N OH

OH .

$\omega = 90$ [1]

III. RESULTS AND DISCUSSION

A , ω_1, ω_2, ω_{12} 40 120 [1] 10 [1] , CNO , F - . O. 9 × 9 × 9 (ω_1, ω_2, ω_{12}) , 729 (3D)- F . , F

F . 5 5 $(\square_1, \square_2, \square_{12})$

. A

: (i, j)

$\rightarrow (i, j+1)$ $j \square 1$

$(i+1, j\ \ 1) \rightarrow (i+1, j)$. N $j \square 2$

$(i+2, j\ \ 2) \rightarrow (i+2, j$

$1)$, . I F . 6

$(\_1, \_2, \_{12})$. S

$\_1$ $(\_2, \_{12})$

. A F 0.5

,

F . 4( ). F

. , 5 ^{1}, F

F

0.60 0.65. C , (12)

.

C. A_1/A_2 plane

A

F $F\,0.985$.

F . 4( ) F

0.987 . I

,

$(\_2, \_{12})$, ,

$\_1$.

$(\_1, \_2, \_{12}) = (40, 50, 50$ $^{1})$, $(50, 90, 90$ $^{1})$,

$(60, 115, 115$ $^{1})$. ,

-

, $\_2$ $\_{12} = 115$ ^{1}, -

, $F = 0.984$. -

F . 7

. N , (i, j)

$\to (i, j+1)$ $j\,1$

$(i+2, j$ $1) \to (i+2, j)$. A F .

6( ) . A

F . 6( ),

$$\square_{12} = \square_2. \quad (13)$$

($\square_1, \square_2, \square_{12}$) ... $\square_1$ ... ($\square_2, \square_{12}$) ... A_1/A_2 ...

F . 4 . A

F . 6 . H

, 10 → 11, 10

→

K , A. M , J. C .