[illegible] st [illegible] f [illegible] s st [illegible] st [illegible] t [illegible] s f A-[illegible] ys [illegible] st-[illegible] s st [illegible] s

[illegible],[1] [illegible],[1,*] [illegible],[2] A [illegible][1,]
[1]N[illegible] R[illegible] E[illegible] L[illegible] G[illegible], C[illegible] 80201, USA
[2]U[illegible] E[illegible]-N[illegible], G[illegible]

(Received 24 [illegible] 2005; [illegible] 15 [illegible] 2006; [illegible] 13 [illegible] 2006)

[illegible]

DOI: 10.1103/[illegible].74.035108 PACS number(s): 61.66.[illegible], 61.50.A[illegible], 81.05.[illegible], 81.30.[illegible]

I. INTRODUCTION

[illegible]

f ... $\mathcal{O}(10)$ ... , f .,
. 50 52)

$$\square H_{LDA}(\square) \equiv E(\square, V_{\square}, \{R \quad x$$

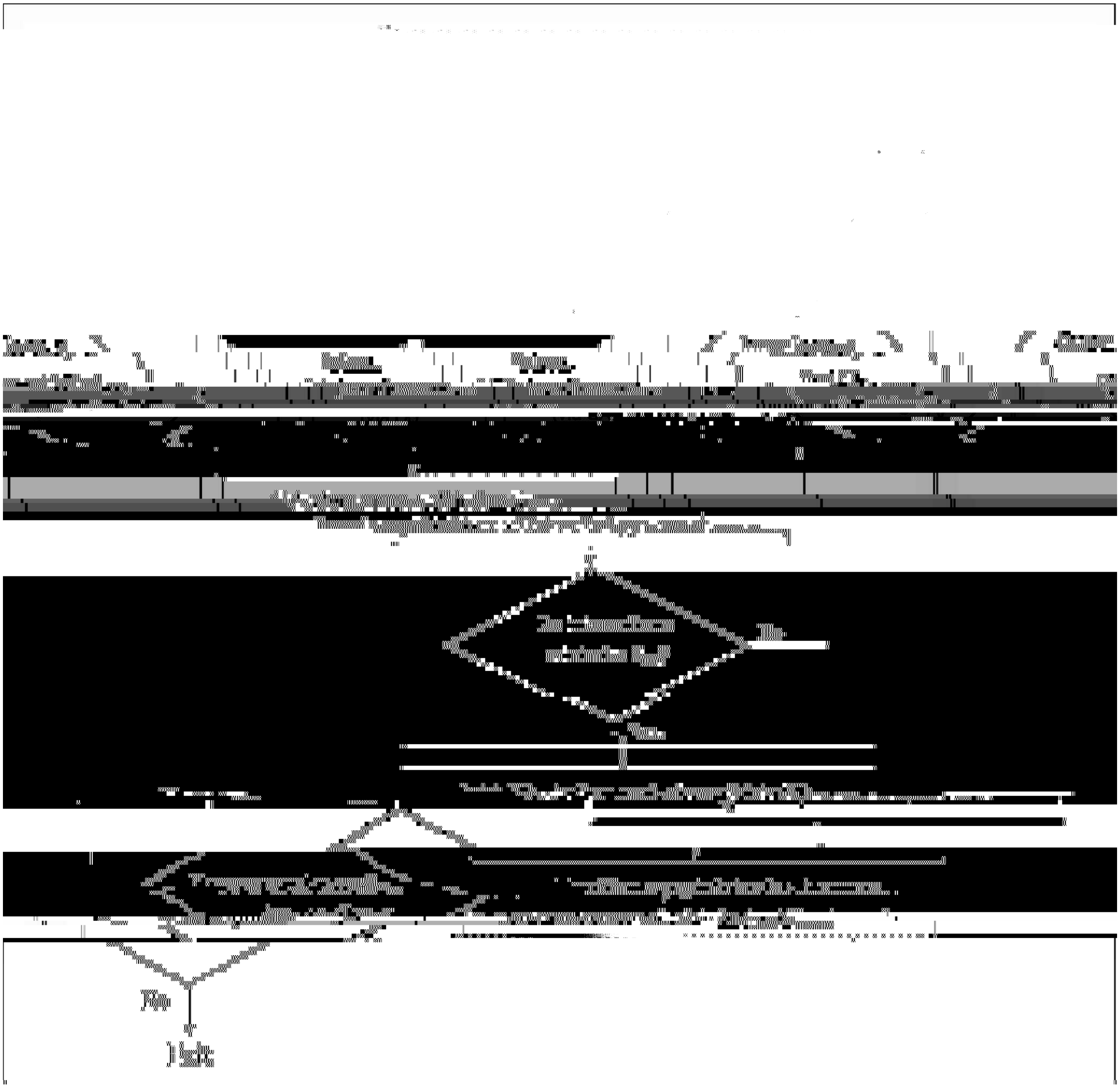

FIG. 3.

[illegible] 66 [illegible] 67. [illegible] $\{H_{LDA}\}$ [illegible] J [illegible] [61] [illegible] [61] [illegible] (5) [illegible]

$$D\,J\,(\ ) = J(\ )|S(\ ,\ )|^2, \quad (7)$$

[illegible] $S(\ ,\ )$ [illegible]

$$MBCE = |H_{LDA}(\ ) - H_{CE}(\ )|^2 + M, \quad (8)$$

$$M = \frac{1}{\square} \quad J(\;)[\;\nabla^2]^{\square/2} J(\;) = \quad R^{\square} D \; J^2 \tag{9}$$

[illegible] (8) [illegible]

. A . . . Ae o ΔH_LDA) A x o ΔH_CE o. A f o ΔH_CE o ΔH_CE .

x	Structure	Description		ΔH_{CE}	ΔH_{LDA}	ΔH_{CE}
		o 2				
1/9	A_8B	(301) A_8B	45.1···	38.5	39.4	38.6
1/6	A_5B	(301) A_5B	59.5···	55.9	57.4	57.3
1/5	A_4B	(201) (301) A_4B	71.3···	67.9	67.3	67.3
5/12	A_7B_5	(302) $A_2B_2A_3B_2A_2B$	91.3···	89.1	93.7	93.7
		o 3				
1/5	$A_{12}B_3$	(301) A_5BABA_6B	71.0···	67.9	67.5	68.5
4/15	$A_{11}B_4$	(401) A_5BABA_4BAB (2 f. 14)	86.6···	84.9	85.4	85.7
2/5	A_9B_6	(401) $A_4B_4A_4BAB$	92.9···	91.6	93.6	89.5
2/3	A_4B_8	(302) $B_5A_2B_3A_2$	69.0···	63.2	58.7	62.4
	A_2B_4	(301) A_2B_4	68.6···	66.4	59.1	58.4
		o 4				
2/11	A_9B_2	(301) A_5BA_4B	64.9···	62.3	62.5	63.9
1/3	$A_{10}B_5$	(401) $A_4BABA_2BA_2BAB$	91.9···	87.8	87.8	87.9
	A_8B_4 (.4905)	(302) $A_5B_2A_3B_2$	95.7···	85.4	91.1	88.2
2/5	A_3B_2	(110) A_2BAB	94.0···	86.7	89.4	89.8
5/8	A_3B_5	(401) B_4A_2BA	75.6···	68.2	64.1	66.6
2/3	A_4B_8	(601) B_6ABA_2BA	68.2···	61.6	60.7	59.7
		o 5				
1/6	$A_{10}B_2$	)	62.2···	54.2	55.3	55.3
1/5	A_8B_2	)	71.5···	66.5	66.5	67.4
1/3	A_8B_4 (.4557)	$A_3BA_2BA_3B_2$ (201)	91.2···	88.8	91.1	90.4
7/12	A_5B_7	(302) $B_2A_2B_3A_2B_2A$	94.4···	91.9	74.8	77.2
		o 6				
1/9	$A_{18}B_2$	)	37.9···	34.8	34.4	35.0
2/17	$A_{15}B_2$	(401) $A_{14}BAB$	43.0···	41.4	41.0	41.3
4/17	$A_{13}B_4$	(401) A_6BABA_5BAB (2 f. 14)	81.5···	78.9	79.9	80.4
1/2	A_3B_3 (.55)	(111) A_3B_3	41.3···	7.4	11.6	11.7
		o 7				
1/11	$A_{10}B$	(301) $A_{10}B_1$	32.7···	31.7	31.4	32.2
2/13	$A_{11}B_2$	(301) A_6BA_5B	54.7···	53.2	53.3	54.6

I. E AND RANGE OF IN ERAC ION REQ IRED FOR DE CRIBING L

A $L1_2$ u f A 3 ($D0_{23}$) A 3 ($L1_2$) f ..., o (α) α = $L1_2$, $D0_{22}$, $D0_{23}$ 12 o 2 fi ( ):

... A B ... A_3B ... AB_3 $L1_2$). ...

... A_3B ... AB_3 ...

... $L1_2$, $D0_{22}$ ... $D0_{23}$ ...

$D0$

$(^{1)} = 10$ $(^{7)} = 8.$ [8]

B. t : t f st t s f st t t CE

1. Ground-state search at different outer-loop iterations

f . 10 f

o =1 =7).

o 16 =1) o 20

=7) o ,

A : f

A

10)] H_{CE}) f

) = 0 A.

f . 4, f

o f

f . 9). =1,

f ,

f

o f . 3)

40% 96 -49 96 -43.19.26285

x			H_{CE}	H_{LDA}

FIG. 10. [illegible] = 1 [illegible] = 7 [illegible]. All [illegible]

[illegible] = 1.

2. Illustrating the outer-loop history

[illegible] Fig. 11 [illegible] $L1_2$ [illegible] ($L1_2/D0_{22}/D0_{23}$) [illegible] Fig. 11, [illegible]

[illegible] = 1 [illegible] Fig. 11 [illegible] = 1 [illegible] = 1.

[illegible] *CE* [illegible] *LDA* [illegible]

[illegible] *CE* [illegible] *LDA* [illegible] $L1_2$ [illegible] = 1 [illegible]

[illegible] *N* [illegible] [301) A_8B [illegible]], [illegible] [301) A_5B [illegible]], [illegible] [301) A_4B [illegible]] [illegible]

[illegible] = 1 [illegible] Fig. 11 [illegible]

[illegible] $L1_2$ [illegible] $L1_2$ [illegible]

[illegible]	[illegible]:	$N=28$ [illegible] =1	$N=32$ [illegible] =2	$N=37$ [illegible] =3	$N=43$ [illegible] =4	$N=47$ [illegible] =5	$N=51$ [illegible] =6	$N=53$ [illegible] =7
[illegible]	A-[illegible] ($D0_{23}$)	0%	88%	92%	62%	64%	100%	100%
[illegible]	A $L1_2/D0_{22}/D0_{23}$ [illegible]	0%	88%	92%	62%	64%	100%	100%
[illegible]	A-[illegible] ($L1_2$)	40%	100%	100%	92%	79%	100%	100%
[illegible]	A $L1_2/D0_{22}/D0_{23}$ [illegible]	0%	37%	100%	85%	79%	100%	100%

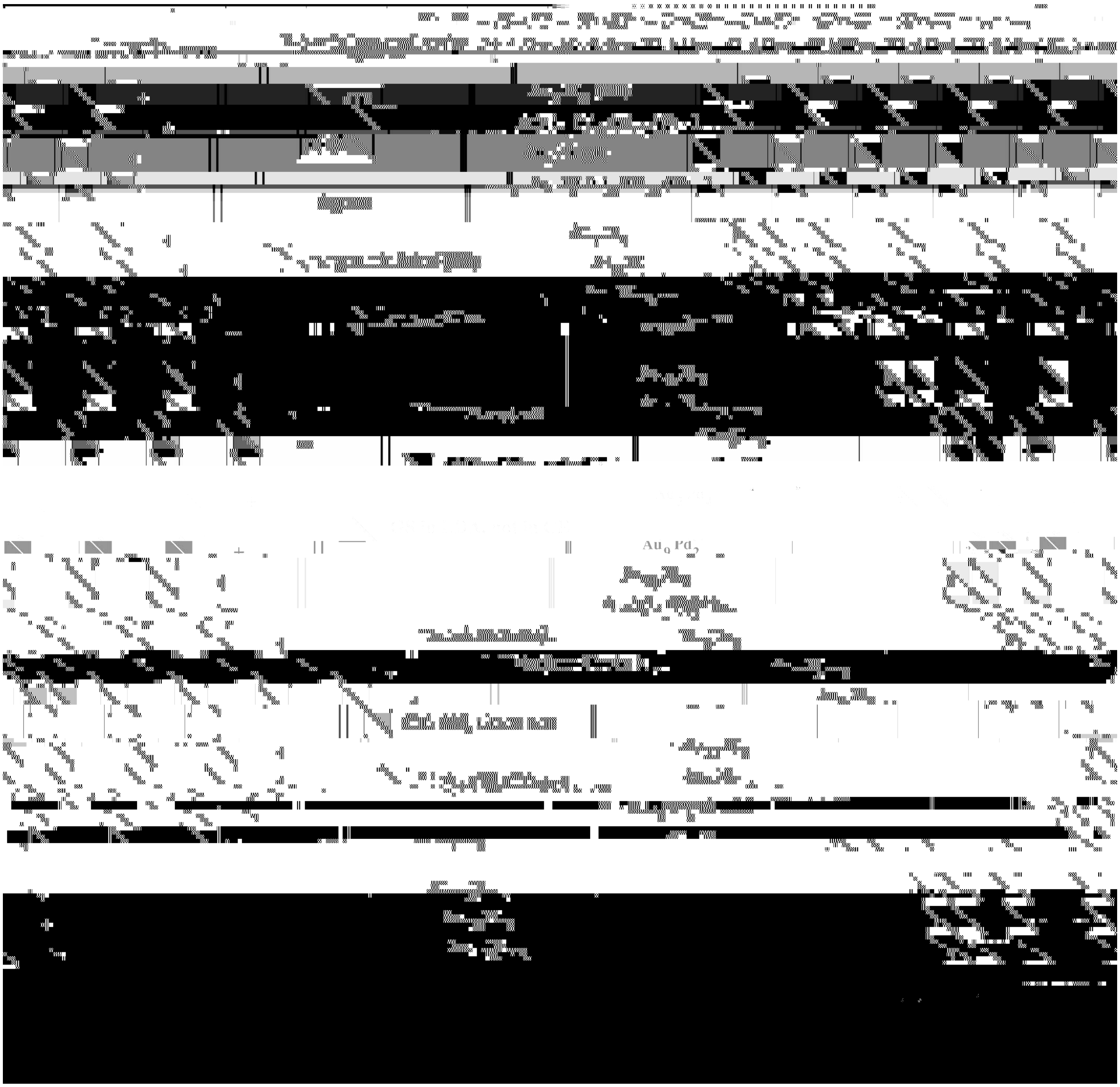

FIG. 11. [illegible]

[illegible]

(a) *CE* [illegible] *LDA* [illegible] Au [illegible] Au$_8$, Au$_5$ [illegible] Au$_7$ 5.

(b) *CE* [illegible] *LDA* [illegible] Au [illegible] Au$_4$ [illegible]

(c) *S* [illegible] *LDA* [illegible] x [illegible].[85] [illegible] H_{LDA} [illegible] Au$_7$ 5, [illegible] Au$_2$ (1) [illegible] Au [illegible].

3. Generic behaviors during outer-loop iterations

[illegible] 11, [illegible]

(a) A [illegible] Au$_3$ $L1_2$.

(b) A [illegible] Au [illegible]

, S_{CV} ... x ... $\{\Delta H_{LDA}\}$ ...

... 37 ... w (ΔH_{LDA}) ...

(ΔH_{CE}) ... f. 13. ... 2.8 ...

II. DI... I... OF GR... ND- ... A E ... RDE... ED- ... C... RE ... IN A$_{1-x}$...$_x$

... A ... A ... f. 14. ...

A. ... A$_{1-x}$...$_x$ ... s, x ... 0.22: (301) " ... t ... st ... t ... s

... [87] ... A ... -A ... [87] ... A ... 301) ... 301) ... A ... f. 14. ... f. 87, ... E_{CS} [... 2) ... f. 12 ( )] ... E_{CS} ... ΔH_{LDA} ... A$_{1-x}$ ... x, f. 12 ( ) ... (001) ... A ... A ...

oo ... [... f. 12 ( )],

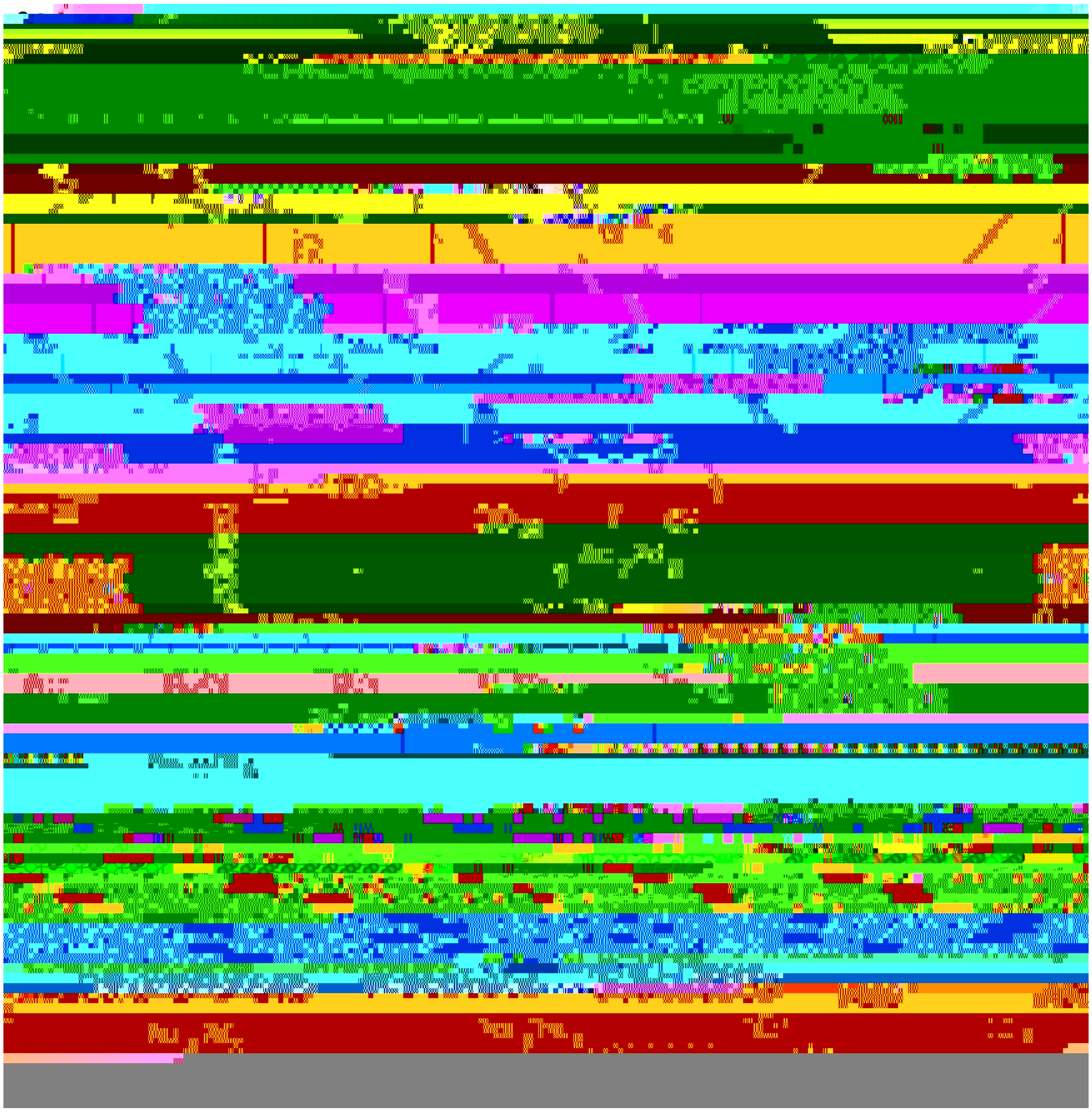

FIG. 14. ... $x \approx 0.22$ ... [10)] ...

... [16] ... 40 ... [57]). ... $x = 1/2$ ... [15] ... [8] ... [89] ... [90] ... [91] ...

... 5 ... $J_0^{(1)}$, $J_0^{(2)}$), ... [8] ... $J_0^{(1)} \approx 0$, ... $J_0^{(2)} \approx 0$, ... $J_0^{(1)}$ ... $J_0^{(2)}/2$ ... A_5B ...

E. D t m s st s : E st t st f -f st t s A

... [15,53] ...

[illegible] N_0 [illegible] 6004 [illegible]

[illegible] N_0 [illegible] 15 [illegible] $N_0 = 176$ [illegible] 3×10^6 [illegible]

[illegible] $x = 1/3$, [illegible] $C37$, [illegible] 15 [illegible] [77,92] [illegible] ~ 10 [illegible] $L1_1$, [illegible] 15 [illegible] $E = 5.463$ [illegible] $E = 5.475$ [illegible] $L1_2$. [illegible] $x = 1/3$. [illegible] ΔH_{LDA} [illegible] 3 [illegible] ΔH_{LDA} ($C37$). [illegible] $C37$ [illegible] $C37$ [illegible] 15 [illegible]

[illegible] [15] [illegible] $D0_{23}$ [illegible] 15, [illegible] ΔH_{LDA} ($L1_2$) [illegible] 12 [illegible] $L1_2$ [illegible] 15 [illegible] $L1_2$ [illegible] T [illegible] $L1_2$ [illegible] ΔH_{LDA} [illegible] $L1_2$ [illegible] 15.

III. CONCLUSION

[illegible]

α

). 80.8 A) 80.5 A) Al_3 $D0_{22}$, 84.0 83.3 Al_3 $D0_{23}$, 97.6 92.6

53.8 49.7 Al_3 $D0_{22}$, 55.6 52.2 Al_3 $L1_2$.

). 11

1

[78] [illegible], 2001.

[79] [illegible] A. **30**, 244 (1944).

[80] [illegible]

[81] [illegible] 1), [illegible] α $D0_{23}$ [illegible] $L1_2$ [illegible] $D0_{22}$. [illegible] $D0_{23}$ [illegible] $L1_2$ 123