THEORETICAL INVESTIGATION OF THE HYDROGEN ELECTRODE REACTION ON (110)-, (100)- AND (111)-LATTICE PLANES OF NICKEL

By

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Abstract

The unidirectional rate i_+ of hydrogen electrode reaction on nickel and the appropriate TAFEL constant $\tau \equiv (RT/F) \cdot (\partial \ln i_+ / \partial \eta)$ were theoretically calculated as a function of overvoltage η at 25°C, 1 atm hydrogen pressure in accordance with the catalytic mechanism as operative on the three principal lattice planes of f.c.c. nickel crystal, *i.e.* (110)-, (100)- and (111)-lattice planes, allowing for the repulsive interactions between hydrogen adatoms and the critical complex of the recombination of hydrogen adatoms, which determines the rate of the reaction.

The lattice planes are assumed to provide respectively congruent lattice planes of sites of hydrogen adatoms and any adjacent pair of the sites composes a seat of the critical complex. It was assumed in the previous investigations[5)7)] that the reaction took place solely on the (110)-lattice plane and that the repulsive potential of hydrogen atom either adsorbed or constituting the critical complex due to surrounding hydrogen adatoms was proportional to the population of the latter (proportional approximation). The rate is now computed by taking account of the repulsive potential due to hydrogen adatoms on sites in the direct neighbourhood of the seat of critical complex statistical mechanically discretely but that due to farther adatoms by the proportional approximation for every lattice plane (combined apppoximation). The evaluation of the rate by the procedure necessitates that of covered fraction θ of sites by hydrogen adatoms and quantities concerned with the repulsion, which are required for the combined approximation, as functions of η.

The results show that (i) the curve of θ plotted against η has each one plateau on the (110)- and (100)-lattice planes, whereas two ones on the (111)-lattice plane, (ii) the (111)-lattice plane contributes predominantly to i_+ or τ over the range of η, where the observation of hydrogen electrode reaction is usually practiced, (iii) the observed $\log i_+ \sim \eta$ or $\tau \sim \eta$ relation[22)] is tolerably reproduced by the theoretical one for $\alpha = 1.5$ by which the exchange repulsive potential calculated as -35% of the MORSE function of hydrogen molecule is multiplied in accordance with an indepen-

dent conclusion of analysis of adsorption isotherms of hydrogen at pressures lower than 1 atm, (iv) the theoretical current density on the (111)-lattice plane decreases with increase of η in the region of $\eta > 0.7$ V and (v) the current density attains finally a constant value on every lattice plane.

The experimental results on $i_+(\eta)$ have previously been theoretically satisfactorily reproduced[7] attributing the seat of reaction solely to the (110)-lattice plane with too large value 4.4 of α, which is now interpreted as just a version of the predominant contribution to $i_+(\eta)$ from the (111)-lattice plane with the reasonable value 1.5 of α.

The above mentioned decrease of i_+ with increase of η on the (111)-lattice plane at high overvoltage is discussed in terms of the increase of repulsive potential of the critical complex due to the closest hydrogen adatoms to the latter (§ 5-3, (4)).

INTRODUCTION

The TAFEL constant τ defined as

$$\tau \equiv \frac{RT}{F}\frac{\partial \ln i_+}{\partial \eta} \qquad (1)$$

is an important characteristic of hydrogen electrode reaction

$$2H^+ + 2e^- = H_2, \qquad (2)$$

where i_+ is the current density representing the forward unidirectional rate of reaction (2), which is practically identical with the observed cathodic current density at sufficiently high an overvoltage η, *i.e.* the cathodic polarization against a reversible hydrogen electrode in the same hydrogen atmosphere and the same electrolyte, H^+ a proton associated with BRÖNSTED base OH^- or H_2O in aqueous solution, e^- a metal electron and F, R or T is of the usual meaning.

It is well-known that τ is, as found by TAFEL[1], *ca.* 0.5 for many metallic cathodes over a considerable range of η.[2)3)] TAFEL himself tried to account for his law, as reviewed briefly below in modern terminology, on the basis of the catalytic mechanism, in which the reaction (2) proceeds through the two steps

$$H^+ + e^- \longrightarrow H(a), \qquad 2H(a) \not\rightarrow H_2, \qquad (3.\,a),\ (3.\,b)$$

the latter being the rate-determining step as signified by $\not\rightarrow$, where H(a) is the hydrogen adatom on the electrode surface. He started[1] from the postulates,

$$i_+ \propto \theta^2, \qquad \theta \propto a, \qquad (4.\,a),\ (4.\,b)$$

where θ is the covered fraction of adsorption sites of hydrogen adatoms on the electrode surface and a the activity of adatom. The chemical potential

$\mu^{H(a)}$ of H(a) is by definition expressed in terms of a as

$$\mu^{H(a)} = RT\ln a + \text{const.}, \tag{5. H}$$

while the partial equilibrium of step (3. a) is stated as

$$\mu^{H^+} + \mu^{e^-} = \mu^{H(a)}, \tag{5. μ}$$

where μ^{H^+} and μ^{e^-} are the chemical (electrochemical) potentials of H^+ and e^- respectively. The μ^{H^+} is a constant for one and the same electrolyte, while μ^{e^-} is given in terms of the particular value $\mu_r^{e^-}$ of μ^{e^-} for the reversible hydrogen electrode and η as

$$\mu^{e^-} = \mu_r^{e^-} + F\eta. \tag{5. e^-}$$

We have from the above three equations

$$a \propto \exp(F\eta/RT), \tag{5. a}$$

hence from Eqs. (4) and (5. a)

$$\ln i_+ = 2F\eta/RT + \text{const.}$$

or $\tau = 2$ according to Eq. (1) in discordance with the experimental results mentioned above.

It has been sometimes accepted that $\tau = 2$ is the criterion of the catalytic mechanism, hence that the observed τ deviating from 2 excludes the mechanism. Attempts have been made on the other hand to reconcile this difference as based on the same mechanism.

The postulate (4. a) is justified on the basis of the LANGMUIR's model[4], provided that interactions among hydrogen atoms on the surface are ignorable. Even on the same basis, however, another postulate (4. b) should be replaced by

$$a \propto \theta/(1-\theta); \tag{6}$$

Eq. (4. b) is the special case of Eq. (6), where θ is negligibly small as compared with unity. It follows from Eqs. (1), (4. a), (5. a) and (6) instead of $\tau = 2$ that

$$\tau = 2\left[1 + \exp\left\{F(\eta - \eta_{1/2})/RT\right\}\right]^{-1}, \tag{7}$$

where $\eta_{1/2}$ is the particular value of η at $\theta = 1/2$. Eq. (7) states that τ decreases continuously from 2 to zero with increase of η, hence transiting the value of 1/2 on its way. However, τ stays around 1/2 for too small an interval of η as compared with experiment, decreasing from 0.8 to 0.2 according to Eq. (7) for only 0.046 V interval of η at 25°C.

OKAMOTO, HORIUTI and HIROTA[5] have shown theoretically that the retention of τ around 0.5 is appreciably improved by the repulsive potentials

between adatoms with each other as well as between the adatoms and constituent atoms of the critical complex of step (3. b), taken into account on the basis of the following model of the electrode. The electrode exposes lattice planes (110) *etc.* and each kind of the lattice planes provides congruent lattice of physically identical sites of hydrogen adatoms, with each site right above a lattice point. Each pair of adjacent sites provides a seat σ^* of the critical complex of rate-determining step (3. b). On the basis of geometry thus defined they estimated the interactions between unbonded atoms, including adatoms, constituent atoms of the critical complex and metal atoms on the lattice planes of nickel crystal in terms of the quantum mechanical exchange potential. They thus obtained the lowest potential of the critical complex on the seat σ^* consisting of a pair of sites $2.49\sqrt{2}$ Å apart from each other on (110)–lattice plane, to which they attributed the predominant contribution to i_+. They have thus calculated i_+ as a function of η arriving at the above result on τ assuming that the repulsive potentials of an adatom and a critical complex due to the surrounding adatoms are respectively proportional to θ.[5] This sort of approximation[6]*) is called the *proportional one* in what follows.

The above treatment is however open to objections. First of all, they attributed the predominant contribution to i_+ to the critical complex of the lowest potential energy without the part due to the repulsion exerted by the surrounding adatoms taken into account, which is not, however, necessarily valid except in case of sparse coverage as demonstrated in the present paper. Second, the repulsive potential of an adatom estimated as the exchange repulsion was too small to account for the decrease of the differential heat of adsorption with increase of θ.[7] Third, the probability $\theta^*(0)$ of a particular σ^* being unoccupied was equated to $(1-\theta)^2$, which is not exact in the presence of the repulsive interaction, where the probabilities of the two constituent sites of σ^* being individually unoccupied are not independent of each other.

One of the present authors[7] has later tried to improve the proportional approximation by multiplying the proportional constants of the repulsive potentials estimated previously[5] as exchange repulsion by a factor $\alpha=4.4$ with reference to an experimental value of heat of adsorption[8], adhering yet to the (110)–lattice plane as the seat of rate-determining step (3. b). The τ was thus found to stay between 0.59 and 0.52 through the increase of η by 0.4 V.

The proportional approximation has turned out theoretically unsatisfactory, on the other hand, on account of the deviation of adsorption isotherm worked out by this approximation from those of higher approximations[9], where the different arrangements of different numbers of adatoms on the first, second and

*) This sort of approximation was applied by BRAGG and WILLIAMS[6] independently.

third nearest sites to that of an adatom of interest, are treated statistical mechanically discretely with regard to repulsions exerted by them in extension of the BETHE-PEIERLS' method[10]. The approximation was called the first, second or third approximation according as the repulsion of surrounding hydrogen adatoms was taken into account statistical mechanically discretely up to the first, second or third nearest neighbours respectively. The isotherms thus obtained appeared to approach an ultimate one with the progress of the degree of approximation, that of the second approximation being found nearly coincident with that of the third approximation, whereas the proportional approximation deviating appreciably from them[9]. The second approximation was thus regarded close enough, while the third approximation was tremendously laborious. TOYA and one of the present authors[11] thus applied the second approximation to fit the theoretical isotherms to the experimental ones with the factor α as a parameter to be adjusted. Results show that the best coincidence of the theoretical isotherms with the experimental ones is obtained for $\alpha \simeq 1.5$[11] in conformity with TOYA's theoretical result[12] that the repulsion must be stronger than the exchange repulsion taken into account by OKAMOTO, HORIUTI and HIROTA.[5] They have suggested[11], however, on the basis of the results obtained that the lattice planes other than (110) have had to be taken into account as well even at pressures of hydrogen less than one atm. In case of cathodic polarization, the other lattice planes may possibly play an important part, since the activity of hydrogen is far higher in this case than that in equilibrium with hydrogen gas at the above mentioned pressure and in consequence the (110)-lattice plane may possibly be fully covered, contributing just a constant, unimportant part to i_+.

The present work is devoted to the theoretical derivation of the $\log i_+ \sim \eta$ relation by a higher approximation taking into account different seats of the critical complex on every principal lattice plane for various values of the factor α to compare the results with observations.

This procedure, if completed, would eliminate all the defects of the previous treatment[5], which costs however an enormous labour. One of the present authors has shown recently[13] that the accuracy of the second approximation of adsorption isotherm is practically attained simply by combining the first and the proportional approximation, *i. e.* by treating the repulsion exerted by the first nearest neighbours to an adatom of interest statistical mechanically discretely, but those exerted by the second and third nearest neighbours by the proportional approximation. This sort of approximation has rendered the calculation of the rates and hence of τ's as a function of η on (110)-, (100)- and (111)-lattice planes respectively for different values of parameter α practicable

along the improved procedure[13], which will be called the *combined appraximation* in what follows.

The rate equation of hydrogen electrode reaction (2) is developed in Chapter I on the basis of the catalytic mechanism. The model of the electrode in the present calculation is defined in Chapter II and the coordinates and the frequencies of normal modes of vibration of the critical complex as well as of hydrogen adatom on the respective lattice planes are determined in Chapter III. The covered fraction θ on the electrode surface and quantities concerned with repulsion are determined in Chapter IV as functions of η. On their bases the current densities and hence τ on the respective lattice planes are calculated and compared with the experiments in the last Chapter.

CHAPTER I. STATISTICAL MECHANICAL FORMULATION OF CATHODIC CURRENT DENSITY

The rate v_+ of a thermal elementary reaction or step is generally expressed as[5)14)]

$$v_+ = \frac{kT}{h}\frac{p^*}{p^{\mathrm{I}}}, \tag{I. 1}$$

identifying the transmission coefficient with unity, where p^* and p^{I} are defined with particular reference to the step (3.b) as follows. Consider a macroscopic assembly C which consists of electrode material, aqueous electrolyte, metal electron and 1 atm hydrogen gas at a definite temperature but comprizes none of the critical complex of the step. The p^* is the factor by which the partition function ΩC of C is multiplied by addition of a critical complex of step (3.b) to C to form C^*, *i. e.*

$$p^* = \Omega C^*/\Omega C, \tag{I. 2. p^*}$$

where ΩC^* is the partition function of C^*. It follows from the properties of partition function, that factor p^* is the BOLTZMANN factor of the free energy increase of C caused by addition of the critical complex to it, *i. e.* that of its chemical potential μ^*,

$$\mu^* = -RT\ln p^*. \tag{I. 2. μ^*}$$

The p^{I} is similarly defined as

$$p^{\mathrm{I}} = \Omega C^{\mathrm{I}}/\Omega C, \tag{I. 2. p^{I}}$$

where ΩC^{I} is the partition function of C^{I}, which is formed by addition of the initial system I of step (3.b), *i. e.* $\mathrm{I}\equiv 2\mathrm{H(a)}$, to C. The factor p^{I} is similarly the BOLTZMANN factor of chemical potential μ^{I} of I and $\mu^{\mathrm{I}}=2\mu^{\mathrm{H(a)}}$ particularly

for the step (3.b), hence

$$2\mu^{H(a)} = -RT\ln p^{I}. \qquad (I.2.\mu^{H(a)})$$

The forward unidirectional current density i_+ of hydrogen electrode reaction (2) is now

$$i_+ = 2e^- \frac{v_+}{A} = 2e^- \frac{kT}{Ah}\frac{p^*}{p^I}, \qquad (I.3)$$

where e^- is the elementary charge and A the area of the electrode, every occurrence of the rate-determining step (3.b) being accompanied by a transfer of two elementary charges in the steady state.

We have from Eqs. (I.2.$\mu^{H(a)}$), (5.H) and (5.a) in the Introduction,

$$-RT\ln p^{I} = 2\mu^{H(a)} = 2F\eta + \text{const.}, \qquad (I.4.I)$$

and const.$=\mu^{H_2}$ since for the reversible hydrogen electrode, $\eta=0$ and $2\mu^{H(a)}=\mu^{H_2}$. We have in consequence

$$p^{I} = \exp\left(-\frac{\mu^{H_2}+2F\eta}{RT}\right)$$

or defining p^{H_2} as $\mu^{H_2}=-RT\ln p^{H_2}$

$$p^{I} = p^{H_2}\cdot\exp\left(-\frac{2F\eta}{RT}\right).$$

The p^{H_2} is now expressed as[14]

$$p^{H_2} = Q^{H_2}/N^{H_2}, \qquad (I.4.H_2)$$

where N^{H_2} is the concentration of hydrogen molecules in gas around the electrode and Q^{H_2} is the partition function of a single hydrogen molecule in gas in unit volume, which is expressed in good approximation[14], identifying the vibrational partition function with unity, as

$$Q^{H_2} = (2\pi mkT)^{3/2}\cdot 4\pi^2 IkTh^{-5}\cdot\exp(-\varepsilon_g^{H_2}/RT), \qquad (I.5.Q^{H_2})$$

where $\varepsilon_g^{H_2}$ is the energy of the ground state of the molecule. We have now from the last three equations

$$p^{I} = \frac{Q^{H_2}}{N^{H_2}}\exp\left(-\frac{2F\eta}{RT}\right) = \frac{(2\pi mkT)^{3/2}}{h^3}\frac{4\pi^2 IkT}{h^2}\times$$
$$\times\exp\left(-\frac{\varepsilon_g^{H_2}}{RT}\right)\exp\left(-\frac{2F\eta}{RT}\right)\cdot\frac{1}{N^{H_2}} \qquad (I.5.I)$$

or according to Eq. (I.2.$\mu^{H(a)}$), defining $p^{H(a)}$ similarly to p^{H_2}, as

$$p^{\mathrm{H(a)}} \equiv \exp\left(-\frac{\mu^{\mathrm{H(a)}}}{RT}\right) = \sqrt{\frac{(2\pi mkT)^{3/2}}{h^3}\frac{4\pi^2 IkT}{h^2}} \times$$
$$\times \exp\left(-\frac{\varepsilon_0^{\mathrm{H_2}}}{2RT}\right)\exp\left(-\frac{F\eta}{RT}\right)\cdot\frac{1}{\sqrt{N^{\mathrm{H_2}}}}. \qquad \text{(I. 5. H)}$$

The p^* as defined by Eq. (I.2.p^*) is expressed as

$$p^* = N^* \frac{\Omega C^*_{\sigma^*(*)}}{\Omega C}, \qquad \text{(I. 6)}$$

where N^* is the total number of seats σ^*'s of the critical complex and $\Omega C^*_{\sigma^*(*)}$ is the partition function of $C^*_{\sigma^*(*)}$ or the particular state of C^* with a single critical complex accommodated in a particular seat σ^*; ΩC^* is in consequence the total sum of $\Omega C^*_{\sigma^*(*)}$'s over all σ^*'s, *i.e.* $N^*\Omega C^*_{\sigma^*(*)}$, in accordance with the premised physical identity*) of σ^*'s of a definite spacing on a definite lattice plane. We have finally from Eqs. (I.3), (I.5.I) and (I.6)

$$i_+ = 2e^- \frac{kT}{h} N_1^* \frac{\Omega C^*_{\sigma^*(*)}}{\Omega C} \frac{N^{\mathrm{H_2}}}{Q^{\mathrm{H_2}}} \exp\left(\frac{2F\eta}{RT}\right), \qquad \text{(I. 7. } i_+\text{)}$$

where

$$N_1^* = N^*/A \qquad \text{(I. 7. } N\text{)}$$

is the number of seats per unit area.

The calculation of i_+ according to Eq. (I.7.i_+) necessitates the evaluation of the factor $\Omega C^*_{\sigma^*(*)}/\Omega C$, which requires in turn the determination of configurations of the critical complex on its seat as in Chapter III.

CHAPTER II. MODEL OF THE ELECTRODE SURFACE

It has been recently shown by TOYA[17] that there exist two types of hydrogen adatoms on metallic adsorbent, *i.e.* r- and s-adatoms as called by him. The r-adatom is an adatom of ordinary sense, *i.e.* that situated outside the electronic surface of the adsorbent forming more or less polarized covalent bond with the latter. The s-adatom is a sort of hydrogen atom dissolved in the adsorbent but situated between the electronic surface and the plane through the outermost metal atoms in an interstitial surface site[15], conducting there quasi two dimentional translation parallel to the electronic surface. There exist one site of r-adatom and another of s-adatom per one metal atom on a lattice plane.[12)15] The r-adatoms repulse each other stronger[15] than the exchange repulsion as estimated by OKAMOTO, HORIUTI and HIROTA[5], while s-adatoms repulse each other as well as r-adatoms to lesser extent.[15] The adsorptions of

*) *Cf.* (c), Chapter II.

r- and s-adatoms may hence occur approximately independent of each other, as assumed in the previous work.[11] The participants of the rate-determining step (3.b) may plausibly be exclusively r-adatoms, as it appears that the recombination of s-adatoms to form hydrogen molecules imbedded in the electron cloud of metal is associated with extremely high an activation energy.

The present treatment is thus simplified by dealing exclusively with r-adatoms allowing for their repulsions, disregarding s-adatoms, on the basis of the following model.

(a) The facets of (110)-, (100)- and (111)-lattice planes are approximately equally developed on the nickel electrode surface.*)

(b) The seat σ^* of the critical complex of step (3.b) consists of a pair of adjacent metal atoms 2.49, $2.49\sqrt{2}$ or $2.49\sqrt{3}$ Å apart from each other on the lattice planes mentioned above, each affording a site σ of hydrogen adatom H(a); three kinds of the seats are all present on (110)-lattice plane, while (111)- or (100)-lattice plane is geometrically devoid of the seat of the second or the third spacing respectively.

(c) The seat σ^*'s of the same spacing or the sites σ's on the same lattice plane are respectively physically identical with each other on a definite lattice plane. Only possible states of σ are practically**) those occupied by one hydrogen adatom or unoccupied.

(d) The MORSE function of H-H, Ni-H or Ni-Ni bond is

$$K+J=D\left[\exp\{-2a(r-r_0)\}-2\exp\{-a(r-r_0)\}\right], \qquad \text{(II. 1)}$$

where K or J is the COULOMB or exchange integral and constants D, a and r_0 shown in Table 1 are respectively the same as those in the previous paper.[5] Table 1 shows also the percentage of the MORSE function comprized by the

TABLE 1. The values of MORSE function.[5]

	a (Å^{-1})	r_0 (Å)	D (Kcal)	Percentage of MORSE Function Comprized by K
H—H	1.98	0.7395	109	10
Ni—H	1.60	1.48	60	24
Ni—Ni	—	—	20	37

*) This postulate is in conformity with the results of low energy electron diffraction[16], field emission microscopy[17] and the conclusion arrived at by one of the present authors and TOYA[11] from analysis of adsorption isotherms that the (110)-lattice plane occupies nearly one third of the BET-surface.

**) It is admitted that the possibility of σ being occupied by a critical complex as a part of σ^* is negligible.

COULOMB integral as calculated in the previous work[5] according to ROSEN and IKEHARA.[18]

CHAPTER III. CONFIGURATION OF CRITICAL COMPLEX

§ 3-1. Coordinates of Constituent Hydrogen Atoms of Critical Complex

Coordinates of constituent hydrogen atoms of the critical complex and its potential energy are determined by the previous method[5] as a four electron problem[19] as below.

Let the coordinates of the two constituent hydrogen atoms, H(1) and H(2) be (x_1,y_1,z_1) and (x_2,y_2,z_2) respectively as shown in Fig. 1. The axis OX is the normal to the lattice plane YZ through the middle point O between two metal atoms, Ni(1) and Ni(2). Positive axis of each coordinate is shown by + sign in parentheses in Fig. 1.

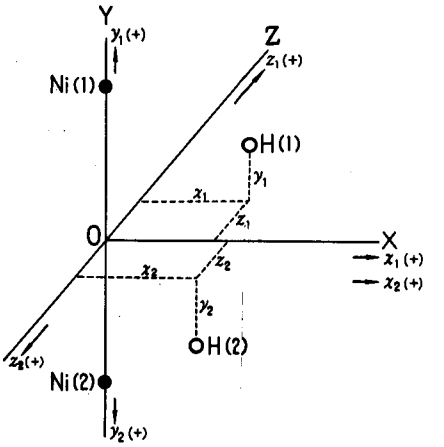

Fig. 1. Coordinates of the two constituent hydrogen atoms of critical complex on a lattice plane represented by YZ.

Introducing new coordinates,

$$x=\frac{x_1+x_2}{2},\quad \xi=\frac{x_2-x_1}{2},$$
$$y=\frac{y_1+y_2}{2},\quad \eta=\frac{y_2-y_1}{2},$$
$$z=\frac{z_1+z_2}{2},\quad \zeta=\frac{z_2-z_1}{2}, \qquad \text{(III. 1)}$$

the potential energy $\varepsilon^{*\prime}$ of the system consisting of Ni(1), Ni(2), H(1) and H(2) is calculated as functions of x and y for $z=\xi=\eta=\zeta=0$*) by the equation[5],

$$\varepsilon^{*\prime}=K_{\mathrm{Ni(1)\text{-}Ni(2)}}+K_{\mathrm{H(1)\text{-}H(2)}}+K_{\mathrm{Ni(1)\text{-}H(1)}}+K_{\mathrm{Ni(1)\text{-}H(2)}}+K_{\mathrm{Ni(2)\text{-}H(1)}}+K_{\mathrm{Ni(2)\text{-}H(2)}}$$
$$-\left[\frac{1}{2}\left\{(J_{\mathrm{Ni(1)\text{-}Ni(2)}}+J_{\mathrm{H(1)\text{-}H(2)}}-J_{\mathrm{Ni(1)\text{-}H(2)}}-J_{\mathrm{Ni(2)\text{-}H(1)}})^2\right.\right.$$
$$\left.\left.+(J_{\mathrm{Ni(1)\text{-}Ni(2)}}+J_{\mathrm{H(1)\text{-}H(2)}}-J_{\mathrm{Ni(1)\text{-}H(1)}}-J_{\mathrm{Ni(2)\text{-}H(2)}})^2+\right.\right.$$

*) The potential energy $\varepsilon^{*}=\varepsilon^{*\prime}+\sum_j(K_j-1/2\cdot J_j)$ inclusive of the repulsive potential $\sum_j(K_j-1/2\cdot J_j)$ of the surrounding metal atoms of number j's, which is eventually used for the calculation of the rate is minimum at this point as seen later.

$$+(J_{\mathrm{Ni(1)\text{-}H(1)}}+J_{\mathrm{Ni(2)\text{-}H(2)}}-J_{\mathrm{Ni(2)\text{-}H(1)}}-J_{\mathrm{Ni(1)\text{-}H(2)}})^2\Big\}\Big]^{1/2}, \qquad \text{(III. 2)}$$

where $K_{\mathrm{Ni(1)\text{-}Ni(2)}}$ *etc.* and $J_{\mathrm{Ni(1)\text{-}Ni(2)}}$ *etc.* are respectively the COULOMB and the exchange integrals, which are evaluated by Eq. (II.1) and Table 1.

The saddle point of the potential energy $\varepsilon^{*\prime}$ for different spacings is determined in order to pick out preliminarily the seat of the critical complex of predominant contribution for each lattice plane as follows. The potential energy surfaces, *i.e.* $\varepsilon^{*\prime}(x,\ y)_{z=\xi=\eta=\zeta=0}$ are illustrated in Figs. 2, 3 and 4 respectively for the spacings 2.49, $2.49\sqrt{2}$ and $2.49\sqrt{3}$ Å of σ^*. Insets of Figs. 2 and 3 illustrate the potential energy near the saddle point. The numerical value of $\varepsilon^{*\prime}(x,\ y)_{z=\xi=\eta=\zeta=0}$ is referred to the energy of the state, where the four atoms involved are at rest infinitely apart from each other. Table 2 shows values x_0 and y_0 respectively of x and y at the saddle point.

The present calculation reproduced the previously calculated[5] coordinates of the saddle point of the critical complex on the seat of $2.49\sqrt{2}$ Å spacing as well as those of the critical complex on the same seat as reported recently

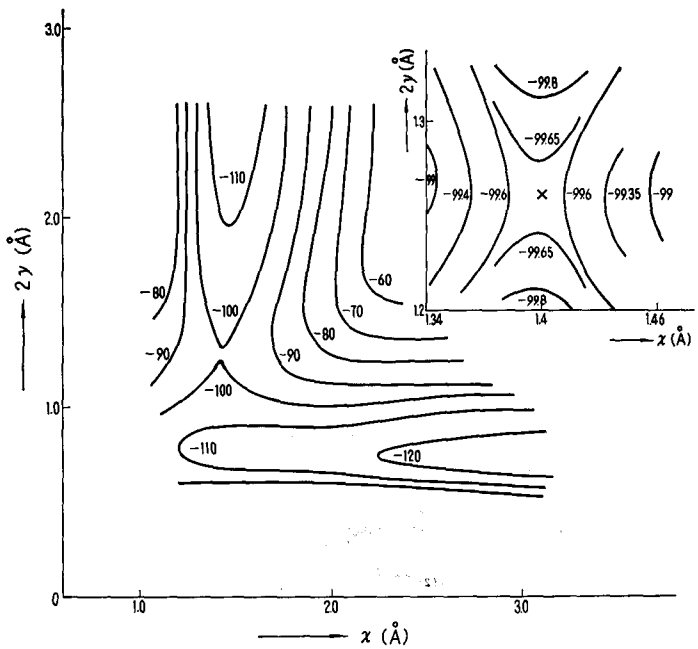

Fig. 2. $\varepsilon^{*\prime}(x,\ y)_{z=\xi=\eta=\zeta=0}$ by Eq. (III.2) for the spacing 2.49 Å of σ^* on Ni. Numerical values are referred to the energy of the state, where four atoms involved are at rest infinitely apart from each other; × indicates the saddle point.

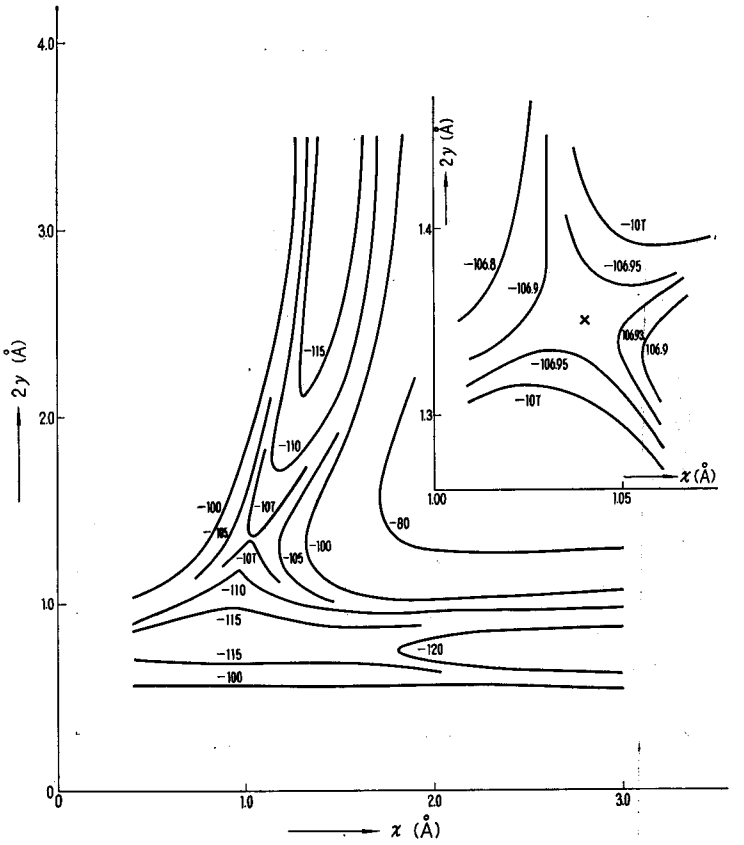

Fig. 3. $\varepsilon^{*\prime}(x, y)_{z=\xi=\eta=\zeta=0}$ by Eq. (III.2) for the spacing $2.49\sqrt{2}$ Å of σ^* on Ni. Numerical values are referred to the energy of the state, where the four atoms involved are at rest infinitely apart from each other; × indicates the saddle point.

by BOCKRIS and SRINIVASAN[20], but not those on the seat of 2.49 Å spacing by the same authors.[20] Actual calculation has shown that the discrepancy is due to the different values of constants, especially of D for Ni–H bond as used in this case by BOCKRIS and SRINIVASAN[20]. The values of $\varepsilon_0^{*\prime}+\sum_j(K_j-1/2\cdot J_j)$ are now determined for the spacings of 2.49, $2.49\sqrt{2}$ or $2.49\sqrt{3}$ Å for each lattice plane by adding*) to $\varepsilon_0^{*\prime}$ ($\varepsilon^{*\prime}$ at the saddle point) the total sum $\sum_j(K_j-1/2\cdot J_j)$ of repulsive potential $K_j-1/2\cdot J_j$ due to j-th metal atom on the lattice plane. Summation was taken over the first nearest metal atoms to those

*) We owe to Dr. T. NAKAMURA for proving the validity of this addition.

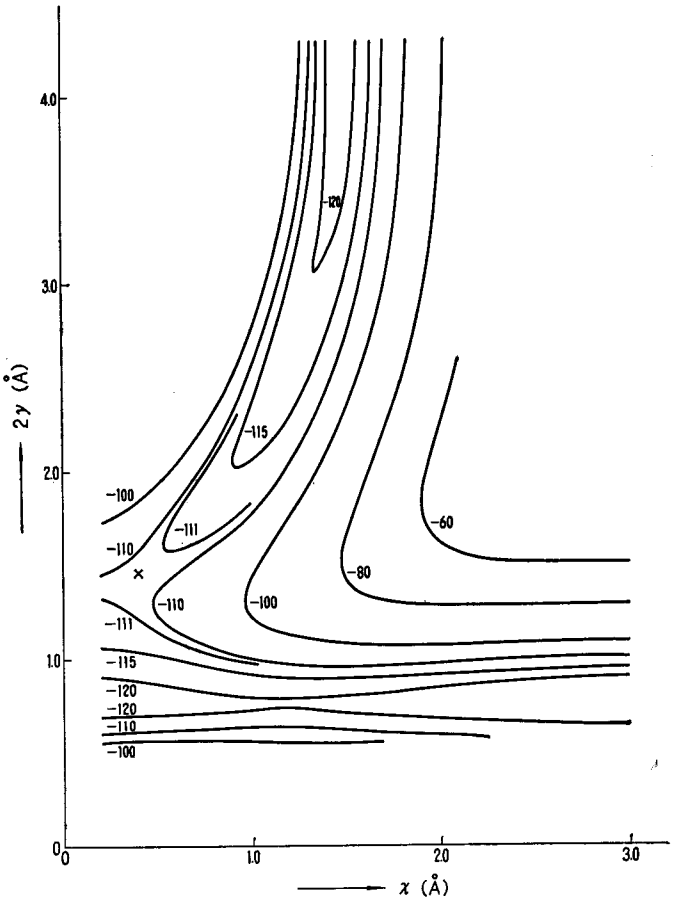

Fig. 4. $\varepsilon^{*\prime}(x, y)_{z=\xi=\eta=\zeta=0}$ by Eq. (III.2) for the spacing $2.49\sqrt{3}$ Å of σ^* on Ni. Numerical values are referred to the energy of the state, where the four atoms involved are at rest infinitely apart from each other.; × indicates the saddle point.

TABLE 2. Configulation of the critical complex.

Ni(1)–Ni(2) distance (Å)	$2y_0$ (Å)	x_0 (Å)
2.49	1.27_0	1.40_0
$2.49\sqrt{2}$	1.35_2	1.04_0
$2.49\sqrt{3}$	1.45	0.400

TABLE 3. Potential energy of the critical complex.

Lattice plane	Distance of Ni-Ni (Å)	$\varepsilon^{*\prime}$ (Kcal)	$\sum_j (K_j - 1/2 \cdot J_j)$ (Kcal)	$\varepsilon_0^{*\prime} + \sum_j (K_j - 1/2 \cdot J_j)$ (Kcal)
(110)	2.49	−99.6	2.3	−97.3
	$2.49\sqrt{2}$	−106.9	8.5	−98.4
	$2.49\sqrt{3}$	−110.6	16.2	−94.4
(100)	2.49	−99.6	9.3	−90.3
	$2.49\sqrt{2}$	−106.9	19.8	−87.1
(111)	2.49	−99.6	9.6	−90.0
	$2.49\sqrt{3}$	−110.6	33.6	−77.1

underlying the relevant seat. The results are shown in Table 3.

The seat of the least value of $\varepsilon_0^{*\prime} + \sum_j (K_j - 1/2 \cdot J_j)$ on each lattice plane is now picked up, *i. e.* that of $2.49\sqrt{2}$, 2.49 or 2.49 Å spacing respectively on (110)-, (100)- or (111)-lattice plane according to Table 3, the further involved calculation being restricted to the latter seat on each lattice plane. This procedure is rather conventional and is desirable of being supplemented or revised in future.

§ 3-2. Determination of Vibrational Frequencies of Critical Complex

Frequencies of the critical complex have to be determined in order to evaluate $\Omega C^*_{\sigma^*(*)}/\Omega C$ as mentioned in Chapter I.

The potential energy ε^* of the critical complex is now expressed inclusive of the repulsive potential $\sum_j (K_j - 1/2 \cdot J_j)$ due to the metal atoms around the relevant σ^* as a function of coordinates of constituent hydrogen atoms of the critical complex, as

$$\begin{aligned}\varepsilon^* = {} & K_{\mathrm{Ni(1)\text{-}Ni(2)}} + K_{\mathrm{H(1)\text{-}H(2)}} + K_{\mathrm{Ni(1)\text{-}H(1)}} + K_{\mathrm{Ni(1)\text{-}H(2)}} + K_{\mathrm{Ni(2)\text{-}H(1)}} + K_{\mathrm{Ni(2)\text{-}H(2)}} \\ & - \Big[\frac{1}{2} \Big\{ (J_{\mathrm{Ni(1)\text{-}Ni(2)}} + J_{\mathrm{H(1)\text{-}H(2)}} - J_{\mathrm{Ni(1)\text{-}H(2)}} - J_{\mathrm{Ni(2)\text{-}H(1)}})^2 \\ & \quad + (J_{\mathrm{Ni(1)\text{-}Ni(2)}} + J_{\mathrm{H(1)\text{-}H(2)}} - J_{\mathrm{Ni(1)\text{-}H(1)}} - J_{\mathrm{Ni(2)\text{-}H(2)}})^2 \\ & \quad + (J_{\mathrm{Ni(1)\text{-}H(1)}} + J_{\mathrm{Ni(2)\text{-}H(2)}} - J_{\mathrm{Ni(2)\text{-}H(1)}} - J_{\mathrm{Ni(1)\text{-}H(2)}})^2 \Big\} \Big]^{1/2} \\ & + \sum_j (K_j - 1/2 \cdot J_j), \end{aligned} \qquad \text{(III. 3)}$$

where the summation of the last term is now extended, as a function of the coordinates of the critical complex, over the first, second and third nearest neighbouring metal atoms to σ^*, *i. e.* those 2.49, $2.49\sqrt{2}$ and $2.49\sqrt{3}$ Å apart

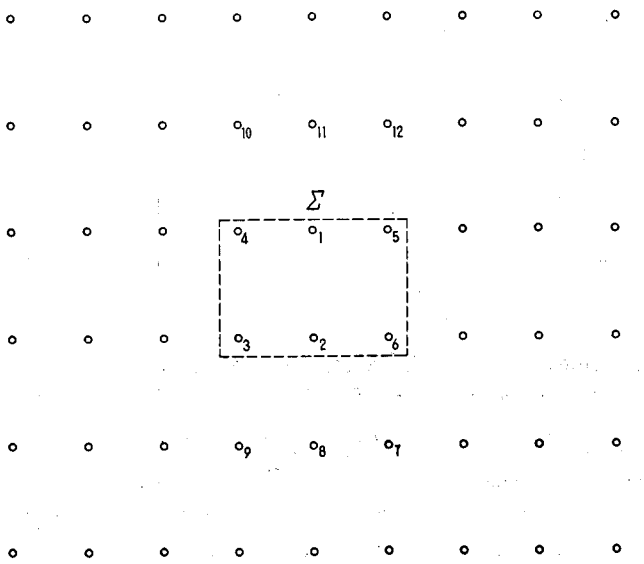

Fig. 5. Arrangement of sites σ's, each provided by a metal atom on (110)-lattice plane. $\sum$ consists of six σ's enclosed by the dotted line, with σ_1 and σ_2 constituting the σ^*.

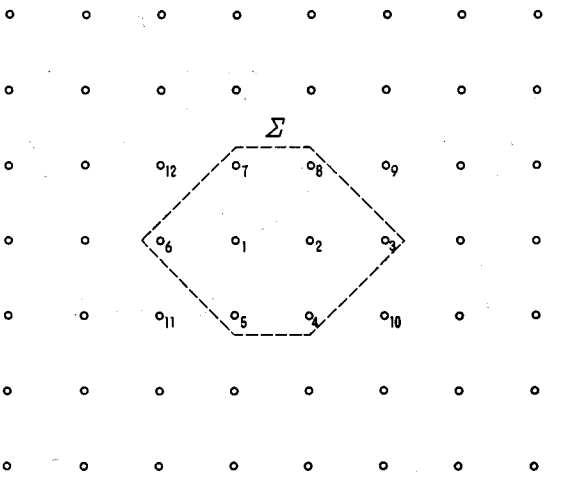

Fig. 6. Arrangement of sites σ's, each provided by a metal atom on (100)-lattice plane. $\sum$ consists of eight σ's enclosed by the dotted line, with σ_1 and σ_2 constituting the σ^*.

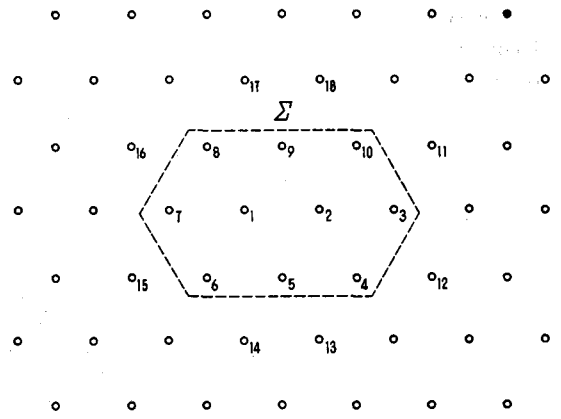

Fig. 7. Arrangement of sites σ's, each provided by a metal atom on (111)-lattice plane. $\sum$ consists of ten σ's enclosed by the dotted line, with σ_1 and σ_2 constituting the σ^*.

from either of the two metal atoms underlying σ^*. These surrounding metal atoms are numbered consecutively from 3 to 12 or 18 as illustrated in Figs. 5, 6 and 7.

The ε^* thus calculated is now expanded in TAYLOR's series around the saddle point*), where $\varepsilon^* = \varepsilon_0^*$, as

$$\varepsilon^* = \varepsilon_0^* + \sum^{x\cdots\xi} \frac{a_{xx}}{2}(x-x_0)^2 + a_{xy}(x-x_0)(y-y_0) + a_{\xi\eta}\xi\eta\,, \qquad \text{(III. 4)}$$

a_{xx} *etc.* represent the force constants. Other cross terms vanish because of the symmetry of the critical complex at the saddle point. The potential energy given above leads to the secular determinants[5];

$$\left.\begin{array}{l} \begin{vmatrix} a_{xx}-2m\lambda & a_{xy} \\ a_{xy} & a_{yy}-2m\lambda \end{vmatrix} = 0\,, \\ \begin{vmatrix} a_{\xi\xi}-2m\lambda & a_{\xi y} \\ a_{\xi y} & a_{\eta\eta}-2m\lambda \end{vmatrix} = 0\,, \\ a_{zz}-2m\lambda = 0 \\ \text{and} \\ a_{\zeta\zeta}-2m\lambda = 0 \end{array}\right\}, \qquad \text{(III. 5)}$$

where $\lambda = 4\pi^2(\nu^*)^2$. The values of ν^* are determined from the roots of the above equations as shown in Table 4. One of the six values is imaginary as signified by the factor $\sqrt{-1}$, which corresponds to the reaction path.

*) The coordinates of the saddle point are found coincident with those of the saddle point of $\varepsilon^{*\prime}$ shown in Table 2.

TABLE 4. Force constants, (a_{xx} *etc.* Kcal mol^{-1} Å^{-2}) and vibrational frequencies (ν^* cm^{-1}) of the critical complex in σ^* of different spacings on different lattice planes of Ni.

	2.49 $\sqrt{2}$ Å, (110)				2.49 Å (100)	2.49 Å (111)	2.49 Å	
	From $\varepsilon^{*\prime}$	BOCKRIS *et al.*[20]	From ε^*	OKAMOTO *et al.*[5]	From ε^*	From ε^*	From $\varepsilon^{*\prime}$	BOCKRIS *et al.*[20]
a_{xx}	230.2	232.75	228.5		348.3	349.3	347.7	−57.55
a_{yy}	−178.8	−155.09	−176.6		−541.0	−541.3	−544.3	546.65
a_{zz}	42.3	0.96	53.5		67.2	71.2	55.2	0.23
$a_{\xi\xi}$	275.0	276.66	273.3		416.0	416.9	415.4	138.69
$a_{\eta\eta}$	277.7	267.09	279.9		100.2	99.9	96.9	26.65
$a_{\zeta\zeta}$	0	38.38	11.2		12.0	16.0	0	124.02
a_{xy}	−195.7	−193.09	−197.1		−39.9	−43.6	−38.2	194.41
$a_{\xi\eta}$	−223.4	−221.30	−224.8		−128.3	−132.0	−126.6	36.23
ν^*		$1170\sqrt{-1}$	$1225\sqrt{-1}$	$839\sqrt{-1}$	$1782\sqrt{-1}$	$1783\sqrt{-1}$		$818\sqrt{-1}$
		1696	1712	1704	1643	1649		1876
		1355	1344	936	1431	1437		933
		543	559	687	627	646		850
		473	551	626	565	552		305
		75	256	368	265	306		36

Table 4 shows the values of force constants derived from $\varepsilon^{*\prime}$ or ε^* in comparison with those previously reported.[5)20)] Those reported by BOCKRIS and SRINIVASAN[20] are coincident with those derived from $\varepsilon^{*\prime}$ except a_{zz} and $a_{\zeta\zeta}$. The value of $a_{\zeta\zeta}$ ought to be zero as derived from $\varepsilon^{*\prime}$ of Eq. (III.2), the relevant mode of motion of the critical complex being just a free rotation. It is also evident that Eq. (III.2) without $\sum_j(K_j - 1/2\cdot J_j)$ makes no difference between force constants of the critical complex on the seat of 2.49 Å spacing on (100)-lattice plane and those on the seat of the same spacing on the (111)-lattice plane. The $a_{\zeta\zeta}$ derived from ε^* of Eq. (III.3) differs from zero as seen in Table 4. The force constants derived from Eq. (III.2) for the seat of 2.49 Å spacing differ from those reported by BOCKRIS and SRINIVASAN as shown in the last two columns in Table 4, which is attributed to the difference of the coordinates of the saddle point due to that of the fundamental constants used in this case as mentioned in §3-1.

The frequencies derived from Eq. (III.3) as given in Table 4 are used in the further calculations.

§ 3–3. Determination of Frequencies of the Hydrogen Adatoms

Vibrational frequencies of hydrogen adatom on the (110)–, (100)– and (111)–lattice planes are determined by the equations,

$$\nu_x = \frac{[(\partial^2\varepsilon^H/\partial x^2)_{x=x_0}]^{1/2}}{2\pi m^{1/2}}, \quad \nu_y = \frac{[(\partial^2\varepsilon^H/\partial y^2)_{y=0}]^{1/2}}{2\pi m^{1/2}}, \quad \nu_z = \frac{[(\partial^2\varepsilon^H/\partial z^2)_{z=0}]^{1/2}}{2\pi m^{1/2}},$$

where m is the mass of hydrogen adatom. Second derivatives are determined from the equation,

$$\varepsilon^H = D_{Ni\text{-}H}\left\{e^{-2a_{Ni\text{-}H}(r-r_0)} - 2e^{-a_{Ni\text{-}H}(r-r_0)}\right\} + \sum_j (K_j - 1/2\cdot J_j),$$

where the last term represents summation of repulsive potentials between the hydrogen adatom and the surrounding metal atoms, *i. e.* the first, second and third nearest neighbours or those 2.49, $2.49\sqrt{2}$ and $2.49\sqrt{3}$ Å apart from the metal atom underlying the relevant site, say σ_1 as shown in Figs. 5, 6 and 7. The numbers of the neighbouring metal atoms taken into account are 8 (those underlying σ_2, σ_3, σ_4, σ_5, σ_6, σ_{10}, σ_{11}, σ_{12} in Fig. 5), 8 (σ_2, σ_4, σ_5, σ_6, σ_7, σ_8, σ_{11}, σ_{12} in Fig. 6) and 12 (σ_2, σ_4, σ_5, σ_6, σ_7, σ_8, σ_9, σ_{10}, σ_{14}, σ_{15}, σ_{16}, σ_{17} in Fig. 7) on (110)–, (100)– and (111)–lattice planes respectively. The values of frequencies thus obtained are listed in Table 5.

TABLE 5. Frequencies ν (cm^{-1}) and $\sum_j (K - 1/2\cdot J_j)$ (Kcal mol^{-1}) of hydrogen adatom.

Lattice plane	ν			$\sum_j (K_j - 1/2\cdot J_j)$
(110)	1898,	79.2,	234	4.57
(100)	1900,	225,	225	8.18
(111)	1901,	248,	248	10.64

CHAPTER IV. ADSORPTION ISOTHERM OF HYDROGEN

Isotherms $\theta = \theta(\eta)$ of hydrogen adatoms are now determined as required to work out $\Omega C^*_{\sigma^*(*)}/\Omega C$ comprized in Eq. (I. 7. *i*) of i_+. The process of the determination is so designed as to yield requisite functions, besides $\theta(\eta)$, for the calculation of $\Omega C^*_{\sigma^*(*)}/\Omega C$ as seen below.

§ 4–1. Fundamentals

Any one of the physically identical sites, σ_i's, on a lattice plane is either

unoccupied or occupied by a hydrogen adatom, which is in partial equilibrium with proton in the electrolyte and metal electron according to the catalytic mechanism as mentioned in Chapter I. Let $C_{\sigma_i(0)}$ or $C_{\sigma_i(\mathrm{H})}$ be the assembly C in the particular state, where σ_i is unoccupied or occupied by a hydrogen adatom respectively with certainty and the $\Omega C_{\sigma_i(0)}$ or $\Omega C_{\sigma_i(\mathrm{H})}$ the respective partition function. It follows that the partition function ΩC of the assembly C without any such specification is the sum of $\Omega C_{\sigma_i(0)}$ and $\Omega C_{\sigma_i(\mathrm{H})}$, *i. e.*

$$\Omega C = \Omega C_{\sigma_i(0)} + \Omega C_{\sigma_i(\mathrm{H})}\,, \tag{IV. 1}$$

while the probability of site σ_i being occupied, is $\Omega C_{\sigma_i(\mathrm{H})}/\Omega C$, common to all sites on a definite lattice plane because of the premised physical identity of sites, which equals the covered fraction θ, *i. e.*

$$\theta = \Omega C_{\sigma_i(\mathrm{H})}/\Omega C\,. \tag{IV. 2. θ}$$

We have from the above two equations,

$$\theta/(1-\theta) = \Omega C_{\sigma_i(\mathrm{H})}/\Omega C_{\sigma_i(0)}\,. \tag{IV. 2. I}$$

Eq. (IV. 2. I) provides the isotherm $\theta = \theta(\eta)$ in question by determining $\Omega C_{\sigma_i(\mathrm{H})}$ and $\Omega C_{\sigma_i(0)}$ as functions of η.

The approximation of $\Omega C_{\sigma_i(\mathrm{H})}$ and $\Omega C_{\sigma_i(0)}$ is schemed for evaluation of the requisite functions as follows. In the combined approximation the repulsion exerted by the first nearest neighbouring hydrogen adatoms to the critical complex is treated statistical mechanically discretely but that exerted by the second and the third nearest ones by the proportional approximation, where the first, second or third nearest neighbouring hydrogen adatom is defined, as in the case of metal atoms in § 3–3, as that located on σ, which is 2.49, $2.49\sqrt{2}$ or $2.49\sqrt{3}$ Å apart from either of the two σ's constituting σ^* of interest. Let now $\sum$ be the group of sites, consisting of a pair of σ's constituting σ^* of interest and the first nearest σ's to the σ^*. Hence $\sum$ includes 6, 8 or 10 σ's as shown enclosed with the dotted line in Fig. 5, 6 or 7, respectively for the (110)–, (100)– or (111)–lattice plane. The partition functions, $\Omega C_{\sigma_i(\mathrm{H})}$ and $\Omega C_{\sigma_i(0)}$ are now developed with special reference to the above defined $\sum$'s in order to evaluate the functions defined below, which are required for the calculation of $\Omega C^*_{\sigma^*(*)}/\Omega C$ as mentioned above.

Let $\Omega C_{\Sigma(0)}$ be the partition function of C at the particular state, where all sites of $\sum$ are unoccupied. By transferring a hydrogen adatom within the assembly from outside $\sum$ onto a definite, unoccupied site σ_i inside $\sum$, the partition function of the assembly is multiplied by a factor $f_{i,\Sigma(0)}$, *i. e.*

$$f_{i,\Sigma(0)} = q^{\mathrm{H(a)}}_{i,\Sigma(0)}/p^{\mathrm{H(a)}}\,, \tag{IV. 3}$$

where $q^{\mathrm{H(a)}}_{i,\Sigma(0)}$ is the factor by which $\Omega C_{\Sigma(0)}$ is multiplied as a hydrogen atom is added to an unoccupied site σ_i inside $\sum$ and $p^{\mathrm{H(a)}}$ is that by which $\Omega C_{\Sigma(0)}$ is multiplied as an adsorbed hydrogen atom is added to the assembly $C_{\Sigma(0)}$, without any specification apart from that all σ's constituting $\sum$ are kept throughout unoccupied.

Let $C_{\Sigma(a)}$ be the assembly at the particular state, where a certain definite set of sites inside $\sum$ are occupied by a definite number of hydrogen adatoms in a definite arrangement signified by $\sum(a)$. The factor $f_{i,\Sigma(a)}$ of multiplication of the partition function $\Omega C_{\Sigma(a)}$ of $C_{\Sigma(a)}$ by transferring a hydrogen adatom within the same assembly from outside $\sum$ onto a definite, unoccupied site σ_i inside $\sum$ of $C_{\Sigma(a)}$ is given in accordance with Eq. (IV.3) by the equation

$$f_{i,\Sigma(a)} = q^{\mathrm{H(a)}}_{i,\Sigma(a)}/p^{\mathrm{H(a)}}, \qquad \text{(IV. 4)}$$

where $q^{\mathrm{H(a)}}_{i,\Sigma(a)}$ is the factor by which $\Omega C_{\Sigma(a)}$ is multiplied by adding a hydrogen adatom onto a definite, unoccupied site σ_i inside $\sum$ of $C_{\Sigma(a)}$.

Now the partition function $\Omega C_{\Sigma(A)}$ of the assembly $C_{\Sigma(A)}$ of a particular population and such arrangement of hydrogen adatoms inside $\sum$ signified by $\sum(A)$ is given by $\Omega C_{\Sigma(0)}$ multiplied by $f_{i,\Sigma(a)}$'s respectively relevant to the successive transfers of hydrogen adatoms to make up $\sum(A)$. The partition function $\Omega C_{\sigma_i(\mathrm{H})}$ or $\Omega C_{\sigma_i(0)}$ of the assembly $C_{\sigma_i(\mathrm{H})}$ or $C_{\sigma_i(0)}$ is now the sum of the $\Omega C_{\Sigma(A)}$'s of $C_{\Sigma(A)}$'s representing respectively all possible numbers of hydrogen adatoms inside $\sum$ in all possible arrangements, compatible with the condition that a definite σ_i inside $\sum$ is kept occupied by a hydrogen adatom or unoccupied respectively with certainty.

The factor $q^{\mathrm{H(a)}}_{i,\Sigma(0)}$ or $q^{\mathrm{H(a)}}_{i,\Sigma(a)}$ defined above is the BOLTZMANN factor of the work required to bring up a hydrogen atom from its standard state onto a definite, preliminarily unoccupied site σ_i inside $\sum(0)$ or $\sum(a)$ to form an adatom there, keeping the assembly involved in statistical mechanical equilibrium throughout (called simply *the reversible work* in what follows). The work mentioned above, *i.e.* $-kT\ln q^{\mathrm{H(a)}}_{i,\Sigma(0)}$ includes the work against the repulsion exerted by hydrogen adatoms outside $\sum$ and $-kT\ln q^{\mathrm{H(a)}}_{i,\Sigma(a)}$ does that of hydrogen adatoms outside as well as inside $\sum$. These parts of the reversible works are identified with the appropriate repulsive potentials.

The repulsive potentials R_{I}, R_{II} and R_{III} are taken α times as large as -35% of the MORSE function of hydrogen molecule, *i.e.* as

$$R_{\mathrm{I}} = 2.346\,\alpha\,,\ R_{\mathrm{II}} = 0.3087\,\alpha\,,\ R_{\mathrm{III}} = 0.0645\,\alpha\ \mathrm{Kcal\,mol^{-1}} \qquad \text{(IV. 5)}$$

for the first, second and third nearest neighbouring hydrogen adatoms, *i.e.* pairs of hydrogen adatoms on sites respectively 2.49, $2.49\sqrt{2}$ and $2.49\sqrt{3}$ Å apart from each other, where α is taken to be 1.2, 1.5 or 2.5; the repulsive

potentials $R_{\mathrm{I},\theta}$ *etc.* due to a single neighbouring adatom are in the proportional approximation assumed to be proportional to θ with the above values of R_{I} *etc.* as proportional constants in the respective cases, *i.e.* as

$$R_{\mathrm{I},\theta} = 2.346\,\alpha\theta\,, \quad R_{\mathrm{II},\theta} = 0.3087\,\alpha\theta\,, \quad R_{\mathrm{III},\theta} = 0.0645\,\alpha\theta \ \mathrm{Kcal\,mol^{-1}}\,. \tag{IV. 6}$$

We now define the following quantities.

(a) The γ is the BOLTZMANN factor of the reversible work required to transfer a hydrogen atom from its adsorbed state outside $\sum$ to its standard state and then from the standard state to a definite, preliminarily unoccupied site inside $\sum$ less the reversible work due to the repulsive interactions with adatoms in the latter process. Hence γ is given as

$$\gamma = q_0^{\mathrm{H(a)}}/p^{\mathrm{H(a)}}\,, \tag{IV. 7. γ}$$

where $q_0^{\mathrm{H(a)}}$ is the BOLTZMANN factor of the reversible work required to transfer a hydrogen atom from its standard state onto a definite, preliminarily unoccupied site inside $\sum$ less the reversible work due to the repulsive interactions with adatoms, which is developed as[5)14)]

$$q_0^{\mathrm{H(a)}} = \prod_{j=1}^{3} \left\{1-\exp(-h\nu_j/kT)\right\}^{-1} \exp(-\varepsilon_g^{\mathrm{H(a)}}/RT)\,; \tag{IV. 7. $q_0^{\mathrm{H(a)}}$}$$

ν_j is the frequency of the j-th normal mode of vibration of the hydrogen adatom and $\varepsilon_g^{\mathrm{H(a)}}$ its energy in the ground state. We have from Eqs. (IV. 7) and (I. 5. H),

$$\gamma = \frac{q_0^{\mathrm{H(a)}}}{p^{\mathrm{H(a)}}} = \sqrt{\frac{N^{\mathrm{H_2}}h^5}{(2\pi mkT)^{3/2}\cdot 4\pi^2 IkT}} \times \prod_{j=1}^{3} \left\{1-\exp\left(-\frac{h\nu_j}{kT}\right)\right\}^{-1} \cdot \exp\left(\frac{1/2\cdot\varepsilon_g^{\mathrm{H_2}} - \varepsilon_g^{\mathrm{H(a)}} + F\eta}{RT}\right). \tag{IV. 8}$$

(b) *I*, *II* or *III* is the BOLTZMANN factor of the repulsive potential R_{I}, R_{II} or R_{III} of Eq. (IV. 5) respectively, *i. e.*

$$I = \exp(-R_{\mathrm{I}}/RT)\,, \quad II = \exp(-R_{\mathrm{II}}/RT) \quad \text{or} \quad III = \exp(-R_{\mathrm{III}}/RT)\,. \tag{IV. 9}$$

(c) I_θ, II_θ or III_θ is the BOLTZMANN factor of the repulsive potential $R_{\mathrm{I},\theta}$, $R_{\mathrm{II},\theta}$ or $R_{\mathrm{III},\theta}$ given by Eq. (IV. 6), *i. e.*

$$I_\theta = \exp(-R_{\mathrm{I},\theta}/RT)\,, \quad II_\theta = \exp(-R_{\mathrm{II},\theta}/RT) \quad \text{or} \quad III_\theta = \exp(-R_{\mathrm{III},\theta}/RT)\,. \tag{IV. 10}$$

(d) The ρ is the BOLTZMANN factor of the repulsive potential between a hydrogen adatom inside $\sum$ and the first nearest hydrogen adatoms outside $\sum$ to it, *i. e.* those on sites 2.49 Å apart from its site. The ρ is determined as shown in §4-2 and used for evaluation of $\Omega C^{\ddagger}_{\sigma^{\ddagger}(\ddagger)}/\Omega C$.

The $f_{i,\Sigma(0)}$ or $f_{i,\Sigma(a)}$ is now expressed in terms of the quantities defined above as*)

$$\left.\begin{aligned} & f_{i,\Sigma(0)} = \gamma \cdot \rho^{l} \cdot II_{\theta}^{s} III_{\theta}^{t} \\ \text{or} \quad & \\ & f_{i,\Sigma(a)} = \gamma \cdot \rho^{l} \cdot I^{u} II^{v} III^{w} \cdot II_{\theta}^{s} III_{\theta}^{t} \end{aligned}\right\}, \qquad \text{(IV. 11)}$$

where l is 1 or 0 according as the site σ_i of interest has first nearest neighbouring site or sites *i. e.* those outside $\sum$ 2.49 Å apart from the σ_i or not and u, v or w is the number of hydrogen adatoms located at the first (2.49 Å), second ($2.49\sqrt{2}$ Å) or third ($2.49\sqrt{3}$ Å) nearest neighbouring sites to σ_i inside $\sum$ and s or t is the number of the second or third nearest sites to σ_i outside $\sum$. These values are determined from the respective spacings of sites and the arrangement of hydrogen adatoms inside $\sum$ as seen in Figs. 5, 6 and 7. The partition function $\Omega C_{\Sigma(A)}$ of the assembly $C_{\Sigma(A)}$ is derived, as stated above, from $\Omega C_{\Sigma(0)}$ multiplying it by $f_{i,\Sigma(a)}$'s respectively relevant to the successive additions of hydrogen adatoms to make up $\sum(A)$. We have hence for a particular population and arrangement $\sum(A)$ of hydrogen adatoms,

$$\Omega C_{\Sigma(A)} = \Omega C_{\Sigma(0)} \prod_{[a]=0}^{[A]-1} f_{i,\Sigma(a)} = \Omega C_{\Sigma(0)} \cdot \gamma^{[A]} \cdot \rho_1^{L} \rho_2^{M} \rho_3^{N} \cdot I^{U} II^{V} III^{W} \cdot II_{\theta}^{S} III_{\theta}^{T}, \qquad \text{(IV. 12)}$$

where $[a]$ or $[A]$ represents the number of adatoms in $\sum$ appropriate to the arrangement $\sum(a)$ or $\sum(A)$ respectively, ρ_1, ρ_2 or ρ_3 is the special case of ρ, where the hydrogen adatom on σ_i inside $\sum$ has one, two or three first nearest (2.49 Å apart) neighbouring sites outside $\sum$, *e. g.* σ_3 in Fig. 5 (ρ_1), σ_5 in Fig. 6 (ρ_2) or σ_6 in Fig. 7 (ρ_3). L, M or N is the total number of the hydrogen adatoms inside $\sum$ associated respectively with the factor ρ_1, ρ_2 or ρ_3. U, V or W is the total number of the pairs of hydrogen adatoms respectively 2.49, $2.49\sqrt{2}$ or $2.49\sqrt{3}$ Å apart from each other inside $\sum$ and S or T is the total number of the pair of hydrogen adatoms $2.49\sqrt{2}$ or $2.49\sqrt{3}$ Å apart from each other, one of them being outside $\sum$ and the other inside $\sum$.

*) The isotherm is worked out here, taking into account the interactions between the second or third nearest ($2.49\sqrt{2}$ or $2.49\sqrt{3}$ Å apart) neighbouring hydrogen adatoms as well as the first nearest ones discretely in case where the neighbours are inside $\sum$. The present approximation as called simply *the higher approximation* of isotherm in what follows is designed as mentioned in the text in order to evaluate the functions ρ_1, ρ_2 and ρ_3 required for the evaluation of $\Omega C^{\ddagger}_{\sigma^{\ddagger}(\ddagger)}/\Omega C$ by the combined approximation.

$\Omega C_{\sigma_i(\mathrm{H})}$ and $\Omega C_{\sigma_i(0)}$ are formulated in the next section using Eq. (IV.12) on the (110)–, (100)– and (111)–lattice planes respectively.

§ 4–2. $\Omega C_{\sigma_i(\mathrm{H})}$, $\Omega C_{\sigma_i(0)}$ and Isotherms

Let $\Omega C_{\sigma_1(\mathrm{H})}$ or $\Omega C_{\sigma_1(0)}$ be the partition function of the assembly $C_{\sigma_1(\mathrm{H})}$ or $C_{\sigma_1(0)}$, where σ_1 in Figs. 5, 6 and 7 is occupied by a hydrogen adatom or unoccupied respectively with certainty.

$\Omega C_{\sigma_1(\mathrm{H})}$ or $\Omega C_{\sigma_1(0)}$ is expressed with reference to $\sum$ as the sum of the partition functions of assemblies for all possible arrangements of every possible number g of hydrogen adatoms inside $\sum$, with σ_1 kept occupied or unoccupied respectively with certainty, *i. e.*

$$\left.\begin{aligned}\Omega C_{\sigma_1(\mathrm{H})} &= \sum_{g=0}^{G} \Omega C_{\Sigma\{\sigma_1(\mathrm{H}),G\sigma(g\,\mathrm{H})\}} \\ \Omega C_{\sigma_1(0)} &= \sum_{g=0}^{G} \Omega C_{\Sigma\{\sigma_1(0),G\sigma(g\,\mathrm{H})\}}\end{aligned}\right\}, \qquad \text{(IV. 13)}$$

where $\Omega C_{\Sigma\{\sigma_1(\mathrm{H}),G\sigma(g\,\mathrm{H})\}}$ or $\Omega C_{\Sigma\{\sigma_1(0),G\sigma(g\,\mathrm{H})\}}$ is the partition function of the assembly in the state, where the σ_1 is occupied by a hydrogen adatom or unoccupied respectively with certainty and the other constituent sites of $\sum$, G in number, *i. e.* 5, 7 or 9 respectively on the (110)–, (100)– or (111)–lattice plane, are occupied by g hydrogen adatoms. Taking into account all possible arrangements of g hydrogen adatoms on G sites, we have

$$\left.\begin{aligned}\Omega C_{\Sigma\{\sigma_1(\mathrm{H}),G\sigma(g\,\mathrm{H})\}} &= \sum_{k(g)} \Omega C_{\Sigma\{\sigma_1(\mathrm{H}),G\sigma(g\mathrm{H})_{k(g)}\}} \\ \Omega C_{\Sigma\{\sigma_1(0),G\sigma(g\,\mathrm{H})\}} &= \sum_{k(g)} \Omega C_{\Sigma\{\sigma_1(0),G\sigma(g\,\mathrm{H})_{k(g)}\}}\end{aligned}\right\}, \qquad \text{(IV. 14)}$$

where $\Omega C_{\Sigma\{\sigma_1(\mathrm{H}),G\sigma(g\,\mathrm{H})_{k(g)}\}}$ or $\Omega C_{\Sigma\{\sigma_1(0),G\sigma(g\mathrm{H})_{k(g)}\}}$ is the partition function of the assembly with further specification that the g hydrogen adatoms inside $\sum$ are in $k(g)$-th arrangement on G sites. The number of the all possible arrangements is $G!/g!(G-g)!$. We have from Eqs. (IV.12), (IV.13) and (IV.14)

$$\left.\begin{aligned}\Omega C_{\sigma_1(\mathrm{H})} &= \sum_{g=0}^{G} \sum_{k(g)=1}^{K(g)} \Omega C_{\Sigma(0)} \cdot \gamma^{g+1} \cdot \left[\rho_1^L \rho_2^M \rho_3^N \cdot I^U II^V III^W \cdot II_\theta^S III_\theta^T\right]_{k(g)} \\ \Omega C_{\sigma_1(0)} &= \sum_{g=0}^{G} \sum_{k(g)=1}^{K(g)} \Omega C_{\Sigma(0)} \cdot \gamma^{g} \cdot \left[\rho_1^L \rho_2^M \rho_3^N \cdot I^U II^V III^W \cdot II_\theta^S III_\theta^T\right]_{k(g)}\end{aligned}\right\}, \qquad \text{(IV. 15)}$$

where $K(g)=G!/g!(G-g)!$ and the values of $L, \cdots, T$ in the parentheses [ ] depend on number $k(g)$ of the arrangement. Eq. (IV.15) is applied to the respective lattice planes as below.

(110)-lattice plane: As illustrated in Fig. 5, there are six σ's in $\sum$ of which four σ's, *i. e.* σ_3, σ_4, σ_5 and σ_6 have only one first nearest (2.49 Å apart) neigh-

bouring site outside $\sum$, whereas σ_2 has none, *i. e.* $G=5$ and $M=N=0$ in Eq. (IV.15), hence

$$\left.\begin{aligned}\Omega C_{\sigma_1(\mathrm{H})} &= \sum_{g=0}^{5}\sum_{k(g)=1}^{K(g)} \Omega C_{\Sigma(0)}\cdot\gamma^{g+1}\cdot\left[\rho_1^L\cdot I^U II^V III^W\cdot II_\theta^S III_\theta^T\right]_{k(g)} \\ \Omega C_{\sigma_1(0)} &= \sum_{g=0}^{5}\sum_{k(g)=1}^{K(g)} \Omega C_{\Sigma(0)}\cdot\gamma^{g}\cdot\left[\rho_1^L\cdot I^U II^V III^W\cdot II_\theta^S III_\theta^T\right]_{k(g)}\end{aligned}\right\}, \quad \text{(IV. 16)}$$

where

$$K(g)=5!/g!(5-g)!\,.$$

All possible arrangements for a given number g of hydrogen adatoms inside $\sum$ and corresponding the terms of the sums in Eq. (IV.16) are listed in Table I in the Appendix, which is transformed into simple forms rearranging the terms into the power series of X as

$$\Omega C_{\sigma_1(\mathrm{H})} = \Omega C_{\Sigma(0)}\left\{\sum_{j=1}^{5}(a_{1,j}\zeta+a_{2,j}\zeta^2)X^{j-1}\right\} \quad \text{(IV. 17. a)}$$

$$\Omega C_{\sigma_1(0)} = \Omega C_{\Sigma(0)}\left\{\sum_{j=1}^{5}(a_{3,j}+a_{4,j}\zeta)X^{j-1}\right\}, \quad \text{(IV. 17. b)}$$

where $X=\gamma\cdot\rho_1\cdot II_\theta III_\theta^3$, $\zeta=\gamma\cdot II_\theta III_\theta^2$ and $a_{k,j}$, $k=1,\cdots,4$ are the constants shown in Table 6. The above equations comprize unknown ρ_1 in X, which is determined by another equation

$$\Omega C_{\sigma_1(0)} = \Omega C_{\sigma_4(0)} \quad \text{(IV. 18. a)}$$

based on the premised physical identity of the sites in accordance with the BETHE-PEIERLS' method, where $\Omega C_{\sigma_4(0)}$ is the partition function of the assembly

TABLE 6. Constants, $a_{k,j}$ in Eqs. (IV.17) for (110)-lattice plane.

k \ j	1	2	3	4	5
1	1	$2I+2III$	$2I\,II\,III+I^2+III^2+2I\,III$	$2I^2II\,III+2I\,II\,III^2$	$I^2II^2III^2$
2	II	$4I\,II\,III$	$2I^2II^2III^2+4I^2II\,III^2$	$4I^3II^2III^3$	$I^4II^3III^4$
3	1	4	$4+2II$	$4II$	II^2
4	1	$2I+2III$	$2I\,II\,III+III^2+I^2+2I\,III$	$2I^2II\,III+2I\,II\,III^2$	$I^2II^2III^2$

$C_{\sigma_4(0)}$, *i. e.* C in the particular state that σ_4 inside $\sum$ is unoccupied with certainty. Eq. (IV.18.a) is written using the expressions of $\Omega C_{\sigma_1(0)}$ and $\Omega C_{\sigma_4(0)}$ given in Table I in the Appendix, as

$$\sum_{j=1}^{5}(b_{1,j}+b_{2,j}\zeta)X^{j-1} = \sum_{j=1}^{5}(b_{3,j}\zeta+b_{4,j}\zeta^2)X^{j-1}, \quad \text{(IV. 18. b)}$$

where $b_{k,j}$, $k=1,\cdots,4$ are constants shown in Table 7.

TABLE 7. Constants, $b_{k,j}$ in Eq. (IV.18.b) for (110)-lattice plane.

k \ j	1	2	3	4	5
1	0	1	$2+II$	$3II$	II^2
2	0	0	0	$I^2II\ III+I\ II\ III^2$	$I^2II^2III^2$
3	1	$I+III$	0	0	0
4	II	$3I\ II\ III$	$I^2II^2III^2+2I^2II\ III^2$	$I^3II^2III^3$	0

We have on the other hand from Eqs. (IV.2.I) and (IV.17),

$$\frac{\theta}{1-\theta}=\frac{\sum_{j=1}^{5}(a_{1,j}\zeta+a_{2,j}\zeta^2)X^{j-1}}{\sum_{j=1}^{5}(a_{3,j}+a_{4,j}\zeta)X^{j-1}}. \qquad \text{(IV. 19)}$$

The θ as well as ρ_1 are now numerically solved as a function of η from the simultaneous equations (IV.18.b) and (IV.19) by the trial and error method for $\alpha=1.2$, 1.5 and 2.5 respectively.

(100)-lattice plane: Here we have eight σ's in $\sum$; two of them *i.e.* σ_3 and σ_6 have three first nearest (2.49 Å apart) sites outside $\sum$ and others have two ones except σ_1 and σ_2, which have none at all and there exists no spacing of $2.49\sqrt{3}$ Å as seen in Fig. 6. Hence, $G=7$ and $L=W=T=0$. Eq. (IV.15) is now

$$\Omega C_{\sigma_1(\mathrm{H})}=\sum_{g=0}^{7}\sum_{k(g)=1}^{K(g)}\Omega C_{\Sigma(0)}\cdot\gamma^{g+1}\cdot\left[\rho_2^M\rho_3^N\cdot I^U II^V\cdot II_\theta^S\right]_{k(g)} \qquad \text{(IV. 20. a)}$$

$$\Omega C_{\sigma_1(0)}=\sum_{g=0}^{7}\sum_{k(g)=1}^{K(g)}\Omega C_{\Sigma(0)}\cdot\gamma^{g}\cdot\left[\rho_2^M\rho_3^N\cdot I^U II^V\cdot II_\theta^S\right]_{k(g)}, \qquad \text{(IV. 20. b)}$$

where

$$K(g)=7!/g!(7-g)!.$$

Table II in the Appendix shows terms of the sums in the above equations for all possible arrangements of hydrogen adatoms of all possible numbers, from which we have finally,

$$\Omega C_{\sigma_1(\mathrm{H})}=\zeta\left[\sum_{j=1}^{5}(a_{1,j}+a_{2,j}Z+a_{3,j}Z^2+a_{4,j}\zeta+a_{5,j}\zeta Z+a_{6,j}\zeta Z^2)\,Y^{j-1}\right] \qquad \text{(IV. 21. a)}$$

$$\Omega C_{\sigma_1(0)}=\sum_{j=1}^{5}\left[(a_{7,j}+a_{8,j}Z+a_{9,j}Z^2+a_{10,j}\zeta+a_{11,j}\zeta Z+a_{12,j}\zeta Z^2)\,Y^{j-1}\right], \qquad \text{(IV. 21. b)}$$

TABLE 8. Constants, $a_{k,j}$ in Eqs. (IV.21) for (100)-lattice plane.

k \ j	1	2	3	4	5
1	1	$2II+2I$	$II^2+2I\,II+I^2+2I^2II$	$2I^2II^2+2I^3II$	I^4II^2
2	I	$4I^2II$	$4I^3II^2+2I^4II^2$	$4I^5II$	I^7II^4
3	$1+I$	$2II^2+2I$ $+2I\,II+2I^2II$	$II^4+3I\,II^2+I^2+4I^2II^2$ $+3I^3II^2$	$2I^2II^4+I^3II^2$ $+2I^3II^3+2I^4II^3$	$I^4II^4+I^5II^4$
4	$2I^2$	$4I^3II+4I^3II^2$	$2I^4II^2+4I^4II^3+2I^4II^4$ $+4I^5II^3$	$4I^6II^4+4I^6II^5$	$2I^8II^6$
5	I	$2I\,II^2+2I^2II$	$I\,II^4+2I^2II^3+I^3II^2$ $+2I^3II^3$	$2I^3II^5+2I^4II^4$	I^5II^6
6	I^3	$4I^4II^2$	$4I^5II^4+2I^6II^4$	$4I^7II^6$	I^9II^8
7	1	4	$4+2I$	$4I$	I^2
8	1	$2II+2I$	$II^2+2I\,II+I^2+2I^2II$	$2I^2II^2+2I^3II$	I^4II^2
9	2	$4+4II$	$2+4II+2II^2+4I\,II$	$4I\,II+4I\,II^2$	$2I^2II^2$
10	$1+I$	$2II^2+2I$ $+2I\,II+2I^2II$	$II^4+3I\,II^2+I^2+4I^2II^2$ $+3I^3II^2$	$2I^2II^4+2I^3II^2$ $+2I^4II^3$	$I^4II^4+I^5II^4$
11	1	$4II$	$4II^2+2I\,II^2$	$4I\,II^3$	I^2II^4
12	I	$2I\,II^2+2I^2II$	$I\,II^4+2I^2II^3+I^3II^2$ $+2I^3II^3$	$2I^3II^5+2I^4II^4$	I^5II^6

where $Y=\gamma\cdot\rho_2\cdot II_\theta^2$, $Z=\gamma\cdot\rho_3\cdot II_\theta^2$, $\zeta=\gamma\cdot II_\theta^2$ and $a_{k,j}$, $k=1,\cdots,12$ are constants shown in Table 8. Two unknowns ρ_2 and ρ_3 respectively comprized in Y and Z are determined by means of another two equations

$$\Omega C_{\sigma_1(0)}=\Omega C_{\sigma_6(0)}\,,\qquad \Omega C_{\sigma_6(0)}=\Omega C_{\sigma_7(0)} \qquad \text{(IV. 22. a), (IV. 22. b)}$$

based on the physical identity of σ's, where $\Omega C_{\sigma_6(0)}$ or $\Omega C_{\sigma_7(0)}$ is the partition function of the assembly $C_{\sigma_6(0)}$ or $C_{\sigma_7(0)}$ in the particular state that σ_6 or σ_7 is unoccupied. Eqs. (IV.22.a) and (IV.22.b) are transformed according to Table II in the Appendix as

$$\sum_{j=1}^{5}(b_{1,j}Z+b_{2,j}Z^2+b_{3,j}\zeta Z^2)\,Y^{j-1}=\sum_{j=1}^{5}(b_{4,j}\zeta+b_{5,j}\zeta^2+b_{6,j}\zeta^2Z)\,Y^{j-1} \qquad \text{(IV. 23. a)}$$

and

$$\sum_{j=1}^{5}(c_{1,j}Z+c_{2,j}\zeta Z+c_{3,j}\zeta^2Z+c_{4,j}Z^2+c_{5,j}\zeta Z^2+c_{6,j}\zeta^2Z^2)\,Y^{j-1}$$
$$=\sum_{j=1}^{5}(c_{7,j}+c_{8,j}\zeta+c_{9,j}\zeta^2+c_{10,j}Z+c_{11,j}\zeta Z+c_{12,j}\zeta^2Z)\,Y^{j-1}\,, \qquad \text{(IV. 23. b)}$$

TABLE 9. Constants, $b_{k,j}$ in Eq. (IV.23.a) for (100)-lattice plane.

k \ j	1	2	3	4	5
1	1	$2+2II$	$1+2II+II^2+2I\,II$	$2I\,II+2I\,II^2$	I^2II^2
2	1	$4II$	$4II^2+2I\,II^2$	$4I\,II^3$	I^2II^4
3	I	$2I\,II^2+2I^2II$	$I\,II^4+2I^2II^3+I^3II^2+2I^3II^3$	$2I^3II^5+2I^4II^4$	I^5II^6
4	1	$2II+2I$	$II^2+2I\,II+I^2+2I^2II$	$2I^2II^2+2I^3II$	I^4II^2
5	I	$4I^2II$	$4I^3II^2+2I^4II^2$	$4I^5II^3$	I^7II^4
6	I^2	$2I^3II+2I^3II^2$	$I^4II^2+2I^4II^3+I^4II^4+2I^5II^3$	$2I^6II^4+2I^6II^5$	I^8II^6

TABLE 10. Constants, $c_{k,j}$ in Eq. (IV.23.b) for (100)-lattice plane.

k \ j	1	2	3	4	5
1	1	$1+II$	0	0	0
2	$1+I$	$II^2+I+I\,II+I^2II$	0	0	0
3	I^2	$I^3II+I^3II^2$	0	0	0
4	1	$3II$	$2II^2+I\,II^2$	$I\,II^3$	0
5	$2I$	$3I\,II^3+3I^2II$	$I\,II^4+2I^2II^3+I^3II^2+2I^3II^3$	$I^3II^5+I^4II^4$	0
6	I^3	$3I^4II^2$	$2I^5II^4+I^6II^4$	I^7II^6	0
7	0	1	$2+I$	$3I$	I^2
8	0	$II+I$	$II^2+2I\,II+I^2+2I^2II$	$3I^2II^2+3I^3II$	$2I^4II^2$
9	0	I^2II	$2I^3II^2+I^4II^2$	$3I^5II^3$	I^7II^4
10	0	0	0	$I\,II+I\,II^2$	I^2II^2
11	0	0	0	$I^2II^4+I^3II^2+I^3II^3+I^4II^2$	$I^4II^4+I^5II^4$
12	0	0	0	$I^6II^4+I^6II^5$	I^8II^6

where $b_{k,j}$, $k=1,\cdots,6$ and $c_{k,j}$, $k=1,\cdots,12$ are constants shown in Tables 9 and 10. We have from Eqs. (IV.23.a) and (IV.23.b) by eliminating Z

$$\frac{-B_2+\sqrt{B_2^2+4B_1B_3}}{2B_1}=\frac{-C_2+\sqrt{C_2^2+4C_1C_3}}{2C_1}, \qquad \text{(IV. 24)*)}$$

where

*) The $-$ sign of the square root is excluded by the condition $Z>0$.

$$B_1 = \sum_{j=1}^{5} (b_{2,j} + b_{3,j}\zeta)\, Y^{j-1},$$

$$B_2 = \sum_{j=1}^{5} (b_{1,j} - b_{6,j}\zeta^2)\, Y^{j-1},$$

$$B_3 = \sum_{j=1}^{5} (b_{4,j}\zeta + b_{5,j}\zeta^2)\, Y^{j-1},$$

$$C_1 = \sum_{j=1}^{5} (c_{4,j} + c_{5,j}\zeta + c_{6,j}\zeta^2)\, Y^{j-1},$$

$$C_2 = \sum_{j=1}^{5} (c_{1,j} + c_{2,j}\zeta + c_{3,j}\zeta^2 - c_{10,j} - c_{11,j}\zeta - c_{12,j}\zeta^2)\, Y^{j-1},$$

and

$$C_3 = \sum_{j=1}^{5} (c_{7,j} + c_{8,j}\zeta + c_{9,j}\zeta^2)\, Y^{j-1}.$$

The covered fraction θ as well as ρ_2 and ρ_3 are now determined by Eqs. (IV.2.I), (IV.21), (IV. 23) and (IV.24) as a function of η by the trial and error method for $\alpha = 1.2$, 1.5 and 2.5 respectively.

(111)-lattice plane: In this case we have ten sites in $\sum$; two of them, σ_5 and σ_9, have each two first nearest (2.49 Å apart) sites outside $\sum$, the others each three ones except σ_1 and σ_2, which have none at all and there exists no spacing of $2.49\sqrt{2}$ Å as seen in Fig. 7, hence $G=9$ and $L=V=S=0$ in Eq. (IV.15) or

$$\Omega C_{\sigma_1(\mathrm{H})} = \sum_{g=0}^{9} \sum_{k(g)=1}^{K(g)} \Omega C_{\Sigma(0)} \cdot \gamma^{g+1} \cdot \left[\rho_2^M \rho_3^N \cdot I^U III^W \cdot III_\theta^T\right]_{k(g)} \qquad \text{(IV. 25. a)}$$

$$\Omega C_{\sigma_1(0)} = \sum_{g=0}^{9} \sum_{k(g)=1}^{K(g)} \Omega C_{\Sigma(0)} \cdot \gamma^{g} \cdot \left[\rho_2^M \rho_3^N \cdot I^U III^W \cdot III_\theta^T\right]_{k(g)}, \qquad \text{(IV. 25. b)}$$

where

$$K(g) = 9!/g!(9-g)!.$$

The terms of the sums in the above equations are shown in Table III in the Appendix, from which we have similarly

$$\Omega C_{\sigma_1(\mathrm{H})} = \zeta \sum_{j=1}^{9} (a_{1,j} + a_{2,j}Z + a_{3,j}Z^2 + a_{4,j}\zeta + a_{5,j}\zeta Z + a_{6,j}\zeta Z^2)\, Y^{j-1} \qquad \text{(IV. 26. a)}$$

$$\Omega C_{\sigma_1(0)} = \sum_{j=1}^{9} (a_{7,j} + a_{8,j}Z + a_{9,j}Z^2 + a_{10,j}\zeta + a_{11,j}\zeta Z + a_{12,j}\zeta Z^2)\, Y^{j-1}, \qquad \text{(IV. 26. b)}$$

where $Y = \gamma \cdot \rho_2 \cdot III_\theta^3$, $Z = \gamma \cdot \rho_3 \cdot III_\theta^4$, $\zeta = \gamma \cdot III_\theta^4$ and $a_{k,j}$, $k = 1, \cdots, 12$ are constants shown in Table 11. Unknowns ρ_2 and ρ_3 comprized in Y and Z are determined by another two equations

TABLE 11. Constants, $a_{k,j}$ in Eqs. (IV.26) for (111)-lattice plane.

k \ j	1	2	3	4	5	6	7
1	1	$3I+2III+1$	$III^3+2I+8I\,III+2I^3$	$3I\,III^3+7I^2III+2I^2III^2+2I^3+4I^3III+I^5III$	$I^2III^4+2I^3III^2+5I^3III^3+4I^4III+I^5III+2I^5III^2$	$I^4III^4+2I^5III^3+I^5III^4+2I^6III^2$	I^7III^4
2	$2I$	$4I\,III+2I^2+4I^2III+2I^3$	$4I^2III+6I^2III^2+2I^3III^3+6I^3III+4I^3III^2+6I^4III+2I^5III$	$2I^3III^2+4I^3III^3+2I^3III^4+12I^4III^2+4I^4III^3+2I^4III^4+10I^5III^2+2I^6III^2+2I^7III^2$	$4I^5III^3+6I^5III^4+2I^5III^5+6I^6III^3+4I^6III^4+6I^7III^3+2I^8III^3$	$4I^7III^5+2I^8III^4+4I^8III^5+2I^9III^4$	$2I^{10}III^6$
3	I^2III	$I^2III^3+2I^3III^2+I^3III^3+2I^4III$	$I^3III^5+2I^4III^3+5I^4III^4+4I^5III^2+I^6III^2+2I^6III^3$	$3I^5III^6+7I^6III^4+2I^6III^5+I^6III^6+2I^7III^3+4I^7III^4+I^9III^4$	$I^7III^8+3I^8III^5+8I^6III^6+I^9III^6+2I^{10}III^5$	$I^{10}III^7+2I^{10}III^8+3I^{11}III^7$	$I^{13}III^9$
4	I	$2I^2+4I^2III$	$I^3+4I^3III+4I^3III^2+2I^3III^3+4I^4III$	$2I^4III^3+4I^4III^4+4I^5III+8I^5III^2+2I^6III^3$	$I^5III^6+4I^6III^4+4I^7III^2+2I^7III^3+4I^7III^4$	$2I^8III^6+4I^9III^4$	$I^{11}III^6$
5	$2I^3$	$8I^4III+4I^5III$	$8I^5III^2+12I^6III^6+4I^6III^3+6I^7III^2$	$8I^7III^3+8I^7III^4+12I^8III^3+4I^8III^4+4I^9III^3+4I^9III^4$	$2I^9III^4+4I^9III^5+2I^9III^6+4I^{10}III^4+12I^{10}III^5+2I^{11}III^4+4I^{11}III^5$	$4I^{12}III^6+4I^{12}III^7+4I^{13}III^6$	$2I^{15}III^8$
6	I^5III	$2I^6III^3+4I^7III^2$	$I^7III^5+4I^8III^4+4I^9III^3+6I^9III^4$	$4I^{10}III^5+2I^{10}III^6+12I^{11}III^5+2I^{12}III^6$	$9I^{13}III^7+2I^{13}III^8+4I^{14}III^7$	$6I^{16}III^9$	$I^{19}III^{11}$
7	1	6	$4I+2III+9$	$12I+6III+2I^2III$	$III^2+4I\,III+4I^2+6I^2III$	$2I^2III^2+4I^3III$	I^4III^2
8	2	$4I+4III+4$	$2+4I+4III+12I\,III+2I^2+2III^2+4I^2III$	$8I\,III+8I\,III^2+12I^2III+4I^2III^2+4I^3III+4I^3III^2$	$8I^2III^2+12I^3III^2+4I^3III^3+6I^4III^2$	$8I^4III^3+4I^5III^3$	$2I^6III^4$
9	II	$4I\,III+2III^3$	$III^5+4I\,III^3+4I^2III+2I^2III^2+4I^2III^3$	$4I^2III^4+4I^2III^5+4I^3III^2+8I^3III^3+2I^4III^4$	$I^4III^3+4I^4III^4+4I^4III^5+2I^4III^6+4I^5III^4$	$2I^6III^5+4I^6III^6$	I^8III^7
10	1	$3I+2III+1$	$3I+8I\,III+I^2III+2I^3+III^3$	$3I\,III^3+7I^2III+2I^2III^2+I^2III^3+2I^3+4I^3III+I^5III$	$I^2III^4+2I^3III^2+5I^3III^3+4I^4III+I^5III+2I^5III^3$	$I^4III^4+2I^5III^3+I^5III^4+2I^6III^2$	I^7III^4
11	$2I$	$4I\,III+4I^2III+2I^2+2I^3$	$4I^2III+6I^2III^2+2I^3III^3+6I^3III+4I^3III^2+6I^4III+2I^5III$	$2I^3III^2+4I^3III^3+2I^3III^4+12I^4III^2+4I^4III^3+2I^4III^4+10I^5III^2+2I^6III^6+2I^7III^2$	$4I^5III^3+6I^5III^4+2I^5III^5+6I^6III^3+4I^6III^4+6I^7III^3+2I^8III^3$	$4I^7III^5+2I^8III^4+4I^8III^5+2I^9III^4$	$2I^{10}III^6$
12	I^2III	$I^2III^3+2I^3III^2+I^3III^3+2I^4III$	$I^3III^5+2I^4III^3+5I^4III^4+4I^5III^2+I^6III^2+2I^6III^3$	$3I^5III^6+7I^6III^4+2I^6III^5+I^6III^6+2I^7III^3+4I^7III^4+I^9III^4$	$I^7III^8+3I^8III^5+8I^8III^6+I^9III^6+2I^{10}III^8$	$I^{10}III^7+2I^{10}III^8+3I^{11}III^7$	$I^{13}III^9$

$$\Omega C_{\sigma_1(0)} = \Omega C_{\sigma_9(0)}, \qquad \Omega C_{\sigma_8(0)} = \Omega C_{\sigma_9(0)}, \qquad \text{(IV. 27. a), (IV. 27. b)}$$

where $\Omega C_{\sigma_8(0)}$ or $\Omega C_{\sigma_9(0)}$ is the partition function of the assembly $C_{\sigma_8(0)}$ or $C_{\sigma_9(0)}$ in the particular state that σ_8 or σ_9 is respectively unoccupied with certainty. Eqs. (IV.27.a) and (IV.27.b) are transformed according to Table III in the Appendix into the forms

$$\sum_{j=1}^{7}(b_{1,j}Z+b_{2,j}Z^2+b_{3,j}\zeta Z^2)Y^{j-1}=\sum_{j=1}^{7}(b_{4,j}\zeta+b_{5,j}\zeta^2+b_{6,j}\zeta^2Z)Y^{j-1} \qquad \text{(IV. 28. a)}$$

and

$$\sum_{j=1}^{7}(c_{1,j}Z+c_{2,j}\zeta Z+c_{3,j}\zeta^2Z+c_{4,j}Z^2+c_{5,j}\zeta Z^2+c_{6,j}\zeta^2Z^2)Y^{j-1}$$
$$=\sum_{j=1}^{7}(c_{7,j}+c_{8,j}\zeta+c_{9,j}\zeta^2+c_{10,j}Z+c_{11,j}\zeta Z+c_{12,j}\zeta^2Z)Y^{j-1}, \qquad \text{(IV. 28. b)}$$

where $b_{k,j}$, $k=1,\cdots,6$ and $c_{k,j}$, $k=1,\cdots,12$ are constants shown in Tables 12 and 13. Eliminating Z from Eqs. (IV.28.a) and (IV.28.b), we have

$$\frac{-B_2+\sqrt{B_2^2+4B_1B_3}}{2B_1}=\frac{-C_2+\sqrt{C_2^2+4C_1C_3}}{2C_1}, \qquad \text{(IV. 29)*)}$$

where

$$B_1=\sum_{j=1}^{7}(b_{2,j}+b_{3,j}\zeta)Y^{j-1},$$

$$B_2=\sum_{j=1}^{7}(b_{1,j}-b_{6,j}\zeta^2)Y^{j-1},$$

$$B_3=\sum_{j=1}^{7}(b_{4,j}\zeta+b_{5,j}\zeta^2)Y^{j-1},$$

$$C_1=\sum_{j=1}^{7}(c_{4,j}+c_{5,j}\zeta+c_{6,j}\zeta^2)Y^{j-1},$$

$$C_2=\sum_{j=1}^{7}(c_{1,j}+c_{2,j}\zeta+c_{3,j}\zeta^2-c_{10,j}-c_{11,j}\zeta-c_{12,j}\zeta^2)Y^{j-1},$$

and

$$C_3=\sum_{j=1}^{7}(c_{7,j}+c_{8,j}\zeta+c_{9,j}\zeta^2)Y^{j-1}.$$

The covered fraction θ as well as ρ_2 and ρ_3 are now determined by Eqs. (IV.2.I), (IV.26), (IV.28) and (IV.29) similarly for $\alpha=1.2$, 1.5 and 2.5 respectively.

§ 4-3. Isotherm by the Proportional Apporximation

Isotherms are calculated by the proportional approximation on the (110)-

*) The − sign of the square root is excluded by the condition $Z>0$.

TABLE 12. Constants, $b_{k,j}$ in Eq. (IV.28.a) for (111)-lattice plane.

k \ j	1	2	3	4	5	6	7
1	1	$2+2III+2I$	$1+2III+III^2+2I+6III+I^2+2I^2III$	$4I\,III+4I\,III^2+6I^2III+2I^3III+2I^3III^2+2I^2III^2$	$4I^2III^2+6I^3III^2+2I^3III^3+3I^4III^2$	$4I^4III^3+2I^5III^3$	I^6III^4
2	III	$4I\,III+2III^3$	$III^5+4I\,III^2+6I^2III+2I^2III^2+2I^3III+2I^3III^2$	$2I^2III^4+4I^2III^5+4I^3III^2+8I^3III^3+2I^4III^4$	$I^4III^3+4I^4III^4+4I^4III^5+2I^4III^6+4I^5III^4$	$2I^6III^5+4I^6III^6$	I^8III^7
3	I^2III	$I^2III^3+2I^3III^2+I^3III^3+2I^4III$	$I^3III^5+2I^4III^3+5I^4III^4+4I^5III^6+2I^6III^3$	$3I^5III^6+7I^6III^4+2I^6III^5+I^6III^6+2I^7III^3+4I^7III^4+I^9III^4$	$I^7III^8+3I^8III^5+8I^8III^6+I^9III^6+2I^{10}III^5$	$3I^{11}III^7+I^{10}III^7+2I^{10}III^8$	$I^{13}III^9$
4	1	$1+2III+3I$	$III^3+3I+8I\,III+I^2III+2I^3$	$3I\,III^3+7I^2III+2I^2III^2+I^2III^3+2I^3+4I^3III+I^5III$	$I^2III^4+2I^3III^2+5I^3III^3+4I^4III+I^5III+2I^5III^6$	$I^4III^4+2I^5III^3+I^5III^4+2I^6III^2$	I^7III^4
5	I	$2I^2+4I^2III$	$I^3+4I^3III+4I^3III^2+2I^3III^3+4I^4III$	$2I^4III^3+4I^4III^4+4I^5III+8I^5III^2+2I^6III^3$	$I^5III^6+4I^6III^4+4I^7III^2+2I^7III^3+4I^7III^4$	$2I^8III^6+4I^9III^4$	$I^{11}III^6$
6	I^3	$4I^4III+2I^5III$	$4I^5III^2+6I^6III^2+2I^6III^3+3I^7III^2$	$4I^7III^3+4I^7III^4+6I^8III^3+2I^8III^4+2I^9III^3+2I^9III^4$	$I^9III^4+2I^9III^5+I^9III^6+2I^{10}III^4+6I^{10}III^5+I^{11}III^4+2I^{11}III^5$	$2I^{12}III^6+2I^{12}III^7+2I^{13}III^6$	$I^{15}III^8$

TABLE 13. Constants, $c_{k,j}$ in Eq. (IV.28.b) for (111)-lattice plane.

k \ j	1	2	3	4	5	6	7
1	1	$1+2III+I$	$III+III^2+2I\,III+I^2III$	$I\,III^2+I^2III^2$	0	0	0
2	$2I$	$3I\,III+I^2$ $+3I^2III+I^3$	$I^2III+4I^2III+I^3III$ $+2I^3III^2+I^4III+I^5III$	0	0	0	0
3	I^3	$3I^4III+I^5III$	$2I^5III^2+2I^6III^2+I^7III^2$	$I^7III^3+I^8III^3$	0	0	0
4	III	$2III^3+3I\,III$	$III^5+3I\,III^3+2I^2III$ $+I^2III^2+3I^2III^3$	$I^2III^4+3I^2III^5+I^3III^2$ $+4I^3III^3+I^4III^4$	$I^4III^4+2I^4III^5+I^4III^6$ $+I^5III^4$	I^6III^6	0
5	$2I^2III$	$2I^2III^3+3I^3III^2$ $+2I^3III^3+3I^4III$	$2I^3III^5+3I^4III^3$ $+7I^4III^4+4I^5III^2$ $+I^6III^2+3I^6III^3$	$4I^5III^6+6I^6III^4+3I^6III^5$ $+I^6III^6+I^7III^3+4I^7III^4$ $+I^9III^4$	$I^7III^8+I^8III^5+6I^8III^6$ $+I^9III^6+I^{10}III^5$	$I^{10}III^8+I^{11}III^7$	0
6	I^5III	$2I^6III^3+3I^7III^2$	$I^7III+3I^8III^4+2I^9III^3$ $+4I^9III^4$	$4I^{10}III^6+5I^{11}III^5+I^{12}III^6$	$3I^{13}III^7+I^{13}III^8$ $+I^{14}III^7$	$I^{16}III^9$	0
7	0	1	$3+III+I$	$4III+5I+I^2III$	$III^2+3I\,III+2I^2$ $+4I^2III$	$2I^2III^2+3I^3III$	I^4III^2
8	0	$III+I$	$III^3+I+6I\,III+I^2III$ $+I^3$	$4I\,III^3+6I^2III+3I^2III^2$ $+I^2III^3+I^3+4I^3III$ $+I^5III$	$2I^2III^4+3I^3III^2$ $+7I^3III^3+4I^4III+I^5III$ $+3I^5III^2$	$2I^4III^4+3I^5III^3$ $+2I^5III^4+3I^6III^2$	$2I^7III^4$
9	0	I^2III	$I^3III+2I^3III^2+I^3III^3$ $+I^4III$	$I^4III^3+3I^4III^4+I^5III$ $+4I^5III^2+I^6III^3$	$I^5III^6+3I^6III^4+2I^7III^2$ $+I^7III^3+3I^7III^4$	$2I^8III^6+3I^9III^4$	$I^{11}III^6$
10	0	0	0	$I\,III+I^2III$	$2I^2III^2+2I^3III^2+I^4III^2$	$3I^4III^3+I^5III^3$	I^6III^4
11	0	0	0	0	$I^5III^3+4I^5III^4+I^6III^3$ $+2I^6III^4+I^7III^3$ $+I^8III^3$	$3I^7III^5+I^8III^4$ $+3I^8III^5+I^9III^4$	$2I^{10}III^6$
12	0	0	0	$I^7III^4+I^8III^4$	$I^9III^5+I^9III^6+2I^{10}III^5$ $+I^{11}III^5$	$I^{12}III^6+2I^{12}III^7$ $+I^{13}III^6$	$I^{15}III^8$

lattice plane just for comparison with isotherms obtained by the higher approximation*) in § 4-2. In the proportional approximation, the seat σ^* of the critical complex is treated as $\sum$ itself, the repulsive potentials due to hydrogen adatoms surrounding the critical complex being altogether smeared out in this case.

The partition function $\Omega C_{\sigma_1(\mathrm{H})}$ and $\Omega C_{\sigma_1(0)}$ of the assembly $C_{\sigma_1(\mathrm{H})}$ and $C_{\sigma_1(0)}$ on the (110)-lattice plane are expressed with reference to the $\sum$ consisting in σ^*, as

$$\Omega C_{\sigma_1(\mathrm{H})} = \Omega C_{\sum\{\sigma_1(\mathrm{H}),\sigma_2(0)\}} + \Omega C_{\sum\{\sigma_1(\mathrm{H}),\sigma_2(\mathrm{H})\}} \qquad \text{(IV. 30. a)}$$

$$\Omega C_{\sigma_1(0)} = \Omega C_{\sum\{\sigma_1(0),\sigma_2(0)\}} + \Omega C_{\sum\{\sigma_1(0),\sigma_2(\mathrm{H})\}} \qquad \text{(IV. 30. b)}$$

or in the form similar to Eq. (IV.15),

$$\Omega C_{\sigma_1(\mathrm{H})} = \Omega C_{\sum(0)}(\gamma \cdot I_\theta^2 II_\theta III_\theta^4 + \gamma^2 \cdot II \cdot I_\theta^4 II_\theta^2 III_\theta^8) \qquad \text{(IV. 31. a)}$$

$$\Omega C_{\sigma_1(0)} = \Omega C_{\sum(0)}(1 + \gamma I_\theta^2 II_\theta III_\theta^4)\,. \qquad \text{(IV. 31. b)}$$

Noting that $\Omega C_{\sigma_1(\mathrm{H})}/\Omega C_{\sigma_1(0)} = \theta/(1-\theta)$, we have from the above two equations

$$\frac{\theta}{1-\theta} = \frac{\gamma \cdot I_\theta^2 II_\theta III_\theta^4 (1 + \gamma \cdot II \cdot I_\theta^2 II_\theta III_\theta^4)}{1 + \gamma \cdot I_\theta^2 II_\theta III_\theta^4}\,. \qquad \text{(IV. 32)}$$

Isotherms are obtained as a function of η by the trial and error method according to Eqs. (IV.32), (IV.8), (IV. 9) and (IV.10) respectively for $\alpha = 0$, 1.0, 1.5, 2.0, 2.5 and 4.4 on the (110)-lattice plane. In case where $\alpha = 0$ or in the absence of repulsion, Eq. (IV.32) is reduced to the equation

$$\frac{\theta}{1-\theta} = \gamma\,. \qquad \text{(IV. 33)}$$

Eq. (IV.33) is equivalent to $\theta = \theta(\eta)$ derived from Eqs. (5.a) and (6) in the Introduction, γ being given as a function of η by Eq. (IV.8), except that the proportional constant is left undetermined in the latter case.

§ 4-4. Calculations and Results

The constants shown in Tables from 6 to 13 are calculated by Eqs. (IV.5) and (IV.9) for $\alpha = 1.2$, 1.5 and 2.5 respectively at 25°C. The γ is now evaluated for a given overvoltage using the values of ν's calculated in § 3-3 (Table 5), $m = 2.016/6.024 \times 10^{23}$ and $I = 4.664 \times 10^{-41}$ g cm^2 [21], at 25°C and 1 atm hydrogen pressure; $(\varepsilon_g^{\mathrm{H(a)}} - 1/2 \cdot \varepsilon_g^{\mathrm{H_2}})$ is taken -12.3 Kcal mol^{-1} for the (110)-lattice plane as determined by analysis of observed isotherms[8] and those for

*) *Cf.* footnote on p. 143.

the other lattice planes are calculated by adding to it the appropriate differences of $\sum_j (K_j - 1/2 \cdot J_j)$ given in Table 5, § 3-3. The values of θ were worked out by the electronic computor, NEAC 2203 G, Nippon Electric Company.

Results of the higher approximation*) of isotherm dealt with in § 4-2 are shown in Fig. 8a and Table 14.

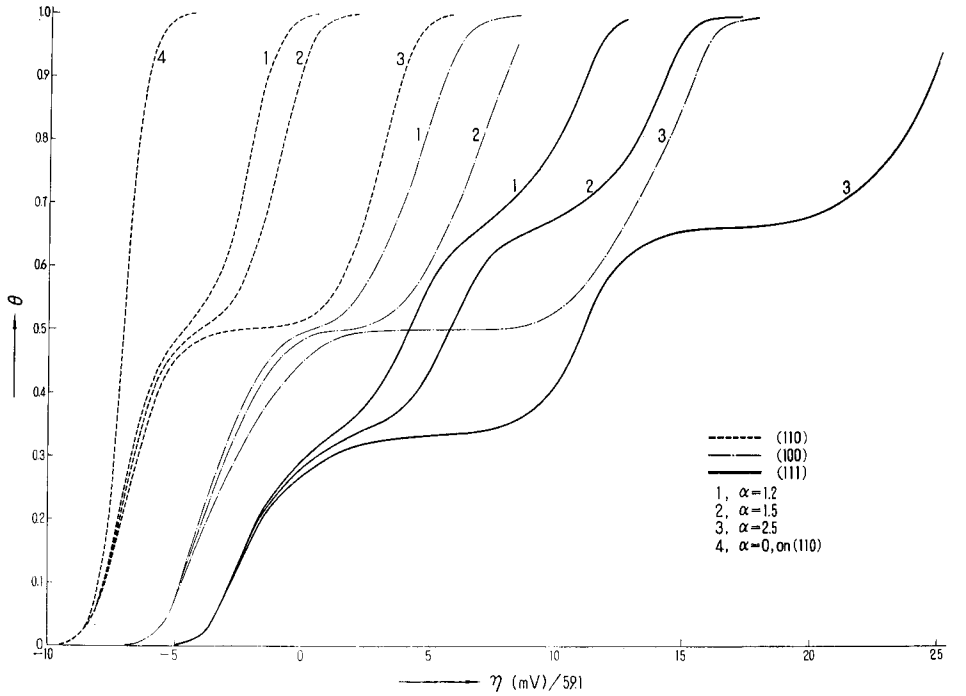

Fig. 8 a. Theoretical isotherms, $\theta = \theta(\eta)$, of hydrogen adsorption on (110)-, (100)- and (111)-lattice planes of Ni by the higher approximation of isotherm for $\alpha = 1.2$, 1.5 and 2.5 at 25°C and 1 atm pressure of hydrogen.

The above results are commented upon as follows.

(1) **Difference due to lattice plane**: Covered fraction θ of the respective lattice planes decreases in the order of (110), (100) and (111) for a given value of overvoltage and α. Fig. 8a shows that the difference of θ due to a definite change of α tends to zero with decrease of θ along with the decrease of repulsive potential. As θ exceeds *ca.* 0.2, on the other hand, the shift of α makes a pronounced difference in θ. Hydrogen adatoms are subject to the strongest repulsion at a given value of θ on the (111)-lattice plane resulting in

*) *Cf.* footnote on p. 143.

TABLE 14. Theoretical values of θ as functions of η at 25°C

Combined Approximation

(110)				(100)				(111)	
$\eta/59.1$	$\alpha=1.2$	$\alpha=1.5$	$\alpha=2.5$	$\eta/59.1$	$\alpha=1.2$	$\alpha=1.5$	$\alpha=2.5$	$\eta/59.1$	$\alpha=1.2$
−9.51	0.0033	0.0033	0.0033	−6.56	0.0049	0.0033	0.0033	−4.71	0.0033
−8.51	0.0291	0.0288	0.0281	−5.56	0.0277	0.0274	0.0268	−3.71	0.0268
−7.51	0.1500	0.1453	0.1331	−4.56	0.1226	0.1192	0.1115	−2.71	0.1095
−6.51	0.3313	0.3206	0.2920	−3.56	0.2461	0.2348	0.2108	−1.71	0.1990
−5.51	0.4457	0.4351	0.4148	−2.56	0.3525	0.3338	0.2898	−0.71	0.2585
−4.51	0.5037	0.4845	0.4719	−1.56	0.4330	0.4130	0.3607	0.29	0.3021
−3.51	0.5664	0.5131	0.4914	−0.56	0.4806	0.4661	0.4196	1.29	0.3366
−2.51	0.6931	0.5595	0.4979	0.44	0.4999	0.4920	0.4626	2.29	0.3718
−1.51	0.8757	0.6679	0.5015	1.44	0.5188	0.4994	0.4866	3.29	0.4278
−0.51	0.9786	0.8417	0.5071	2.44	0.5656	0.5048	0.4969	4.29	0.5145
0.49	0.9977	0.9665	0.5235	3.44	0.6455	0.5236	0.4996	5.29	0.5935
1.49	0.9998	0.9961	0.5722	4.44	0.7515	0.5690	0.4999	6.29	0.6401
2.49	0.9999	0.9996	0.6847	5.44	0.8748	0.6409	0.5000	7.29	0.6733
3.49	0.9999	0.9999	0.8429	6.44	0.9712	0.7351	0.5001	8.29	0.7107
4.49	0.9999	0.9999	0.9622	7.44	0.9966	0.8462	0.5006	9.29	0.7588
5.49	0.9999	0.9999	0.9953	8.44	0.9997	0.9540	0.5040	10.29	0.8264
				9.44			0.5160	11.29	0.9222
				10.44			0.5428	12.29	0.9857
				11.44			0.5886	13.29	
				12.44			0.6496	14.29	
				13.44			0.7218	15.29	
				14.44			0.8030	16.29	
				15.44			0.9049	17.29	
				16.44			0.9801	18.29	
				17.44			0.9977	19.29	
				18.44			0.9998	20.29	
				19.44			0.9999	21.29	
				20.44			0.9999	22.29	
				21.44			0.9999	23.29	
								24.29	
								25.29	

and 1 atm pressure of hydrogen on different lattice planes.

		Proportional Approximation						No Interaction	
(111)		(110)						(110)	
$\alpha=1.5$	$\alpha=2.5$	$\eta/59.1$	$\alpha=1.0$	$\alpha=1.5$	$\alpha=2.0$	$\alpha=2.5$	$\alpha=4.4$	$\eta/59.1$	$\alpha=0$
0.0033	0.0032	−9.51	0.003	0.003	0.003	0.003	0.003	−9.51	0.003
0.0267	0.0263	−7.51	0.108	0.089	0.076	0.067	0.047	−8.51	0.032
0.1079	0.1043	−5.51	0.412	0.308	0.248	0.209	0.134	−8.01	0.096
0.1951	0.1879	−3.51	0.746	0.558	0.444	0.370	0.231	−7.71	0.174
0.2511	0.2409	−2.51	0.887					−7.51	0.250
0.2901	0.2770	−1.51	0.972	0.800	0.642	0.534	0.330	−7.31	0.346
0.3175	0.3031	−0.51	0.996	0.904				−7.11	0.456
0.3373	0.3190	0.49		0.973	0.833	0.697	0.428	−6.91	0.571
0.3576	0.3272	1.49		0.996	0.915			−6.71	0.678
0.3918	0.3315	2.49			0.973	0.854	0.526	−6.51	0.770
0.4601	0.3344	3.49			0.996	0.923		−6.31	0.841
0.5515	0.3377	4.49				0.974	0.624	−6.11	0.893
0.6142	0.3434	5.49				0.996		−5.91	0.930
0.6452	0.3550	6.49					0.723	−5.71	0.955
0.6647	0.3800	8.49					0.821	−5.51	0.971
0.6850	0.4341	10.49					0.914	−5.31	0.981
0.7146	0.5254	12.49					0.985	−5.11	0.988
0.7561	0.5995	13.49					0.997	−4.91	0.993
0.8155	0.6355	14.49						−4.71	0.995
0.9055	0.6522	15.49							
0.9794	0.6601								
0.9976	0.6638								
0.9998	0.6660								
0.9999	0.6700								
0.9999	0.6757								
0.9999	0.6874								
0.9999	0.7091								
	0.7419								
	0.7856								
	0.8531								
	0.9432								

the smallest θ at a given overvoltage. It may be noted that the (110)-lattice plane is covered almost completely as seen in Fig. 8a at overvoltage above *ca.* 0.2 V, where the hydrogen electrode reaction are usually observed. This point is discussed in §5-3.

(2) **Shape of isotherms**: One or two plateaus appear in isotherms on every lattice plane in the higher approximation, whereas not at all in the proportional approximation as seen in Fig. 8b. The appearance of the plateaus may be

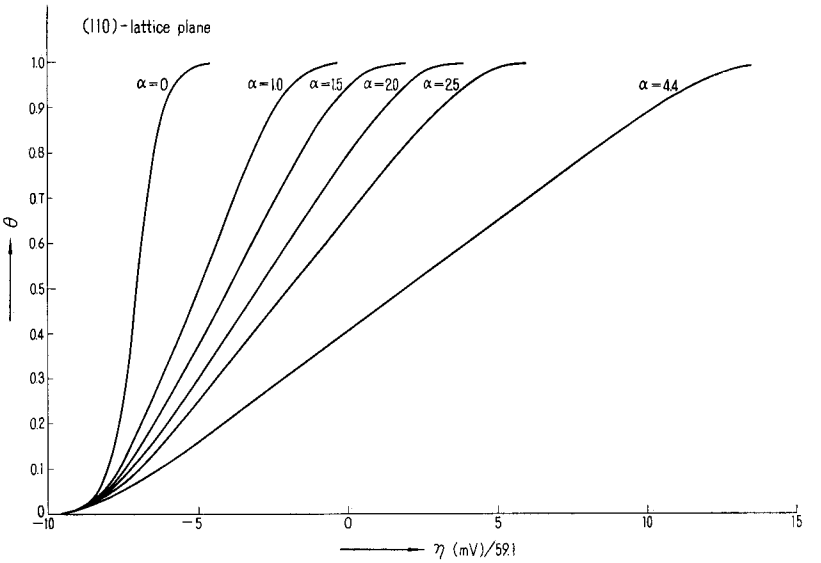

Fig. 8b. Theoretical isotherms, $\theta=\theta(\eta)$, of hydrogen adsorption on (110)-lattice plane of Ni by the proportional approximation for $\alpha=1.0$, 1.5, 2.0, 2.5 and 4.4 at 25°C and 1 atm pressure of hydrogen.

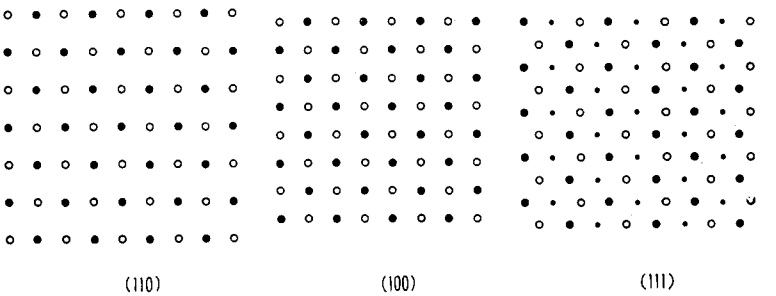

Fig. 9. Adsorption of hydrogen on (110)-, (100)- and (111)-lattice planes. Adsorption occurs first on the sites of solid circle and then on those of open circle. The sites marked by points are occupied in the last stage of adsorption on account of the strongest repulsion.

understood as follows. With increase of η or of activity of hydrogen adatom, the sites signified by solid circle in Fig. 9 ought to be first covered on account of the smallest repulsion thus effected. As these sites are covered completely, θ is 1/2 on the (110)- and (100)-lattice planes or 1/3 on the (111)-lattice plane, although only approximately realized except at 0°K. Further occupation of the other sites indicated by open circle in Fig. 9 encounters now with much stronger repulsion, thus giving rise to a hindrance of θ increase or a plateau on the isotherm as seen in Fig. 8a. The length of plateau depends on the extent of the repulsion, *i.e.* longer plateau for larger value of α. As η becomes large enough to overcome this repulsion, θ starts again to increase. The sites on the (111)-lattice plane, marked by point are occupied only in the last stage of increased η on account of the extremely strong repulsion as seen in Fig. 9.

(3) **Comparison of isotherms**: The isotherms obtained by the proportional approximation are illustrated in Fig. 8b and in Table 14. Striking difference is found between the latter results and those of the higher approximation of isotherm shown in Fig. 8a. In the absence of interactions ($\alpha=0$), the electrode surface is completely covered at very low overvoltages, which lie far below those where actual observations are practiced[22]. The coverage obtained for $\alpha=4.4$ on (110)-lattice plane increases from 0 to 1, as seen in Fig. 8b, through an appreciably wide range of overvoltage, covering the region of actual observations of hydrogen electrode reaction. It must be mentioned that the value of $\alpha=4.4$ is far too large as compared with the value of $\alpha\simeq1.5$[11] obtained previously from the analysis of hydrogen isotherm as referred to in Chapter V.

The values of X, Y and Z are shown in Table 15, which are used in the calculation of reaction rate and TAFEL constant in the next Chapter.

CHAPTER V. RATES AND TAFEL CONSTANTS

The rates of hydrogen electrode reaction and its TAFEL constant are now calculated on (110)-, (100)- and (111)-lattice planes by the combined approximation and compared with experimental results. The proportional approximation is conducted on the (110)-lattice plane only for comparison inclusive of the case of no interaction.

§ 5-1. Rates and TAFEL Constant

The rate i_+ of hydrogen electrode reaction is calculated by Eq. (I.7.i_+) for the catalytic mechanism, *i.e.*

$$i_+ = 2e^- \frac{kT}{h} N_1^* \frac{\Omega C_{\sigma^*(*)}^*}{\Omega C} \frac{N^{H_2}}{Q^{H_2}} \cdot \exp\left(\frac{2F\eta}{RT}\right). \qquad \text{(I. 7. } i_+\text{)}$$

TABLE 15. Values of X, Y and

(110)				(100)				
$\eta/59.1$	X			$\eta/59.1$	Z			
	$\alpha=1.2$	$\alpha=1.5$	$\alpha=2.5$		$\alpha=1.2$	$\alpha=1.5$	$\alpha=2.5$	$\alpha=1.2$
−9.51	$3.317\cdot10^{-3}$	$3.315\cdot10^{-3}$	$3.306\cdot10^{-3}$	−6.56	$3.300\cdot10^{-3}$	$3.298\cdot10^{-3}$	$3.293\cdot10^{-3}$	$3.311\cdot10^{-3}$
−8.51	$3.146\cdot10^{-2}$	$3.124\cdot10^{-2}$	$3.057\cdot10^{-2}$	−5.56	$3.006\cdot10^{-2}$	$2.993\cdot10^{-2}$	$2.955\cdot10^{-2}$	$3.095\cdot10^{-2}$
−7.51	$2.361\cdot10^{-1}$	$2.299\cdot10^{-1}$	$2.119\cdot10^{-1}$	−4.56	$1.869\cdot10^{-1}$	$1.842\cdot10^{-1}$	$1.771\cdot10^{-1}$	$2.210\cdot10^{-1}$
−6.51	1.222	1.176	1.043	−3.56	$6.980\cdot10^{-1}$	$6.755\cdot10^{-1}$	$6.202\cdot10^{-1}$	1.094
−5.51	4.871	4.691	4.240	−2.56	2.261	2.163	1.815	4.430
−4.51	1.724·10	1.633·10	1.502·10	−1.56	6.855	7.045	6.036	1.619·10
−3.51	6.160·10	5.466·10	4.948·10	−0.56	1.470·10	1.984·10	2.038·10	6.209·10
−2.51	$2.530\cdot10^{2}$	$1.892\cdot10^{2}$	$1.588\cdot10^{2}$	0.44	2.005·10	3.552·10	6.521·10	$2.137\cdot10^{2}$
−1.51	$1.378\cdot10^{3}$	$7.440\cdot10^{2}$	$5.060\cdot10^{2}$	1.44	2.720·10	4.199·10	$1.924\cdot10^{2}$	$7.321\cdot10^{2}$
−0.51	$1.089\cdot10^{4}$	$3.721\cdot10^{3}$	$1.620\cdot10^{3}$	2.44	5.772·10	4.740·10	$4.039\cdot10^{2}$	$2.810\cdot10^{3}$
0.49	$1.047\cdot10^{5}$	$2.662\cdot10^{4}$	$5.305\cdot10^{3}$	3.44	$1.744\cdot10^{2}$	7.268·10	$5.002\cdot10^{2}$	$1.027\cdot10^{4}$
1.49	$1.043\cdot10^{6}$	$2.486\cdot10^{5}$	$1.850\cdot10^{4}$	4.44	$5.646\cdot10^{2}$	$1.860\cdot10^{2}$	$5.159\cdot10^{2}$	$4.143\cdot10^{4}$
2.49	$1.042\cdot10^{7}$	$2.466\cdot10^{6}$	$7.336\cdot10^{4}$	5.44	$2.093\cdot10^{3}$	$5.939\cdot10^{2}$	$5.189\cdot10^{2}$	$2.039\cdot10^{5}$
3.49	$1.042\cdot10^{8}$	$2.464\cdot10^{7}$	$3.480\cdot10^{5}$	6.44	$1.287\cdot10^{4}$	$1.923\cdot10^{3}$	$5.226\cdot10^{2}$	$1.444\cdot10^{6}$
4.49	$1.042\cdot10^{9}$	$2.464\cdot10^{8}$	$2.267\cdot10^{6}$	7.44	$1.167\cdot10^{5}$	$6.494\cdot10^{3}$	$5.450\cdot10^{2}$	$1.346\cdot10^{7}$
5.49	$1.042\cdot10^{10}$	$2.464\cdot10^{9}$	$2.041\cdot10^{7}$	8.44	$1.154\cdot10^{6}$	$3.385\cdot10^{4}$	$7.189\cdot10^{2}$	$1.336\cdot10^{8}$
				9.44			$1.636\cdot10^{3}$	
				10.44			$4.926\cdot10^{3}$	
				11.44			$1.589\cdot10^{4}$	
				12.44			$5.402\cdot10^{4}$	
				13.44			$1.762\cdot10^{5}$	
				14.44			$5.145\cdot10^{5}$	
				15.44			$1.929\cdot10^{6}$	
				16.44			$1.260\cdot10^{7}$	
				17.44			$1.163\cdot10^{8}$	
				18.44			$1.153\cdot10^{9}$	
				19.44			$1.152\cdot10^{10}$	
				20.44			$1.152\cdot10^{11}$	
				21.44			$1.152\cdot10^{12}$	

Z on different lattice planes.

(100)			(111)					
Y		$\eta/59.1$	Z			Y		
$\alpha=1.5$	$\alpha=2.5$		$\alpha=1.2$	$\alpha=1.5$	$\alpha=2.5$	$\alpha=1.2$	$\alpha=1.5$	$\alpha=2.5$
$3.309\cdot10^{-3}$	$3.303\cdot10^{-3}$	−4.71	$3.301\cdot10^{-3}$	$3.300\cdot10^{-3}$	$3.295\cdot10^{-3}$	$3.313\cdot10^{-3}$	$3.312\cdot10^{-3}$	$3.308\cdot10^{-3}$
$3.082\cdot10^{-2}$	$3.042\cdot10^{-2}$	−3.71	$3.020\cdot10^{-2}$	$3.009\cdot10^{-2}$	$2.977\cdot10^{-2}$	$3.118\cdot10^{-2}$	$3.109\cdot10^{-2}$	$3.083\cdot10^{-2}$
$2.177\cdot10^{-1}$	$2.086\cdot10^{-1}$	−2.71	$1.957\cdot10^{-1}$	$1.934\cdot10^{-1}$	$1.876\cdot10^{-1}$	$2.316\cdot10^{-1}$	$2.296\cdot10^{-1}$	$2.241\cdot10^{-1}$
1.066	$9.951\cdot10^{-1}$	−1.71	$7.924\cdot10^{-1}$	$7.770\cdot10^{-1}$	$7.474\cdot10^{-1}$	1.228	1.212	1.181
4.275	3.950	−0.71	2.488	2.396	2.294	5.226	5.120	5.055
1.510·10	1.385·10	0.29	7.168	6.619	6.244	1.987·10	1.882·10	1.873·10
5.361·10	4.403·10	1.29	2.203·10	1.738·10	1.585·10	7.571·10	6.515·10	6.291·10
$2.253\cdot10^{2}$	$1.371\cdot10^{2}$	2.29	6.129·10	4.434·10	3.810·10	$3.304\cdot10^{2}$	$2.301\cdot10^{2}$	$2.022\cdot10^{2}$
$7.241\cdot10^{2}$	$4.561\cdot10^{2}$	3.29	$2.487\cdot10^{2}$	$1.160\cdot10^{2}$	8.799·10	$2.033\cdot10^{3}$	$8.971\cdot10^{2}$	$6.420\cdot10^{2}$
$2.068\cdot10^{3}$	$1.662\cdot10^{3}$	4.29	$2.072\cdot10^{3}$	$3.721\cdot10^{2}$	$1.962\cdot10^{2}$	$2.539\cdot10^{4}$	$4.409\cdot10^{3}$	$2.045\cdot10^{3}$
$8.599\cdot10^{3}$	$5.901\cdot10^{4}$	5.29	$1.357\cdot10^{4}$	$2.284\cdot10^{3}$	$4.212\cdot10^{2}$	$2.502\cdot10^{5}$	$4.084\cdot10^{4}$	$6.582\cdot10^{3}$
$3.195\cdot10^{4}$	$2.095\cdot10^{4}$	6.29	$4.841\cdot10^{4}$	$4.660\cdot10^{4}$	$9.068\cdot10^{2}$	$1.335\cdot10^{6}$	$1.223\cdot10^{6}$	$2.166\cdot10^{4}$
$1.107\cdot10^{5}$	$7.501\cdot10^{4}$	7.29	$1.420\cdot10^{5}$	$2.478\cdot10^{5}$	$2.049\cdot10^{3}$	$5.481\cdot10^{6}$	$9.919\cdot10^{6}$	$7.466\cdot10^{4}$
$4.258\cdot10^{5}$	$2.641\cdot10^{5}$	8.29	$4.020\cdot10^{5}$	$7.660\cdot10^{5}$	$4.509\cdot10^{3}$	$2.055\cdot10^{7}$	$4.667\cdot10^{7}$	$2.827\cdot10^{5}$
$1.939\cdot10^{6}$	$9.461\cdot10^{5}$	9.29	$1.167\cdot10^{6}$	$2.008\cdot10^{6}$	$1.551\cdot10^{4}$	$8.004\cdot10^{7}$	$1.785\cdot10^{8}$	$1.303\cdot10^{6}$
$1.220\cdot10^{7}$	$3.355\cdot10^{6}$	10.29	$3.853\cdot10^{6}$	$5.172\cdot10^{6}$	$7.781\cdot10^{4}$	$3.609.10^{8}$	$6.248\cdot10^{8}$	$9.698\cdot10^{6}$
	$1.431\cdot10^{7}$	11.29	$1.779\cdot10^{7}$	$1.357\cdot10^{7}$	$4.401\cdot10^{7}$	$2.113\cdot10^{9}$	$2.166\cdot10^{9}$	$7.824\cdot10^{9}$
	$4.667\cdot10^{7}$	12.29	$1.333\cdot10^{8}$	$3.741\cdot10^{7}$	$4.602\cdot10^{8}$	$1.734\cdot10^{10}$	$8.078\cdot10^{9}$	$1.192\cdot10^{11}$
	$1.451\cdot10^{8}$	13.29		$1.171\cdot10^{8}$	$1.668\cdot10^{9}$		$3.500\cdot10^{10}$	$6.483\cdot10^{11}$
	$4.659\cdot10^{8}$	14.29		$4.952\cdot10^{8}$	$4.474\cdot10^{9}$		$1.925\cdot10^{11}$	$2.644\cdot10^{12}$
	$1.667\cdot10^{9}$	15.29		$3.397\cdot10^{9}$	$1.052\cdot10^{10}$		$1.487\cdot10^{12}$	$9.450\cdot10^{12}$
	$6.749\cdot10^{9}$	16.29		$3.166\cdot10^{10}$	$2.162\cdot10^{10}$		$1.417\cdot10^{13}$	$3.162\cdot10^{13}$
	$3.368\cdot10^{10}$	17.29		$3.141\cdot10^{11}$	$3.832\cdot10^{10}$		$1.409\cdot10^{14}$	$1.025\cdot10^{14}$
	$2.454\cdot10^{11}$	18.29		$3.139\cdot10^{12}$	$1.148\cdot10^{11}$		$1.408\cdot10^{15}$	$3.286\cdot10^{14}$
	$2.310\cdot10^{12}$	19.29		$3.139\cdot10^{13}$	$2.620\cdot10^{11}$		$1.408\cdot10^{16}$	$1.043\cdot10^{15}$
	$2.294\cdot10^{13}$	20.29		$3.139\cdot10^{14}$	$6.121\cdot10^{11}$		$1.408\cdot10^{17}$	$3.320\cdot10^{15}$
	$2.293\cdot10^{14}$	21.29		$3.139\cdot10^{15}$	$1.488\cdot10^{12}$		$1.408\cdot10^{18}$	$1.084\cdot10^{16}$
	$2.293\cdot10^{15}$	22.29			$3.828\cdot10^{12}$			$3.805\cdot10^{16}$
	$2.293\cdot10^{16}$	23.29			$1.078\cdot10^{13}$			$1.515\cdot10^{17}$
		24.29			$3.675\cdot10^{13}$			$7.164\cdot10^{17}$
		25.29			$1.831\cdot10^{14}$			$4.433\cdot10^{18}$

The TAFEL constant is expressed according to Eqs. (1) and (I.7.i_+) as

$$\tau = 2 + \frac{RT}{F}\frac{\partial}{\partial \eta}\ln\frac{\Omega C^{*}_{\sigma^{*}(*)}}{\Omega C}\,. \qquad \text{(V. 1)}$$

$\Omega C^{*}_{\sigma^{*}(*)}/\Omega C$ needs now to be evaluated as a function of η on the respective lattice planes.

§ 5-2. $\Omega C^{*}_{\sigma^{*}(*)}/\Omega C$

The configuration of critical complex has already been determined in Chapter III on which basis the repulsive potential between a hydrogen adatom and the pair of constituent hydrogen atoms of the critical complex is calculated, assuming the repulsive potential to be α times as large as -35% of the MORSE function of Eq. (II.1), similarly to R_{I} *etc.* in Eq. (IV.5). We see from Fig. 5 that any hydrogen adatom on one of the first nearest sites to σ^{*} in $\sum$, *i.e.* σ_3, σ_4, σ_5 and σ_6 is equally apart from the constituent atoms of the critical complex on the (110)-lattice plane, which is not the case on the (100)- and (111)-lattice planes as seen from Figs. 6 and 7. The relevant repulsive potentials, R^{*}_{I} *etc.* are calculated in Kcal mol^{-1} as

$$\left.\begin{aligned} &R^{*}_{\mathrm{I}} = 1.721\,\alpha && && \text{(110)-lattice plane,}\\ &R^{*}_{\mathrm{I}} = 0.7652\,\alpha\,, && R^{*}_{\mathrm{II}} = 2.708\,\alpha && \text{(100)-lattice plane,}\\ &R^{*}_{\mathrm{I}} = 0.7652\,\alpha\,, && R^{*}_{\mathrm{II}} = 1.349\,\alpha\,, && \text{(111)-lattice plane,}\\ &R^{*}_{\mathrm{III}} = 7.484\,\alpha && && \end{aligned}\right\} \qquad \text{(V. 2)}$$

where R^{*}_{I} is the repulsive potential between the critical complex and a hydrogen adatom on σ_3 of each lattice planes, R^{*}_{II} that on σ_4 of the (100)- and (111)-lattice planes and R^{*}_{III} that on σ_5 of the (111)-lattice plane respectively. The repulsive potential of critical complex due to the adatoms on the second and third nearest neighbouring sites to σ^{*} lying outside $\sum$ is taken as mentioned in §4-1 to be proportional to the coverage θ in the combined approximation, the appropriate proportional constants R^{*}_{θ} being evaluated as the total sum of the repulsive potentials at $\theta = 1$ calculated by the same law, as

$$R^{*}_{\theta} = 0.1091\,\alpha\theta\,, \quad 0.5015\,\alpha\theta \quad \text{or} \quad 0.2386\,\alpha\theta \ \text{Kcal mol}^{-1}$$

respectively for (110)-, (100)- or (111)-lattice plane. The BOLTZMANN factor of R^{*}_{I}, R^{*}_{II}, R^{*}_{III} or R^{*}_{θ} is denoted by $\boldsymbol{I}$, $\boldsymbol{II}$, $\boldsymbol{III}$ or ζ^{*} respectively.

$\Omega C^{*}_{\sigma^{*}(*)}$: $\Omega C^{*}_{\sigma^{*}(*)}$ is expressed, similarly to $\Omega C_{\sigma_1(\mathrm{H})}$ in the foregoing Chapter, by the combined approximation, as

$$\Omega C^{*}_{\sigma^{*}(*)} = \sum_{g=0}^{G}\sum_{k(g)=1}^{K(g)} \Omega C_{\Sigma(0)} \cdot q_0^{*}\zeta^{*} \cdot \gamma^{g} \times$$
$$\times \left[\rho_1^{L}\rho_2^{M}\rho_3^{N} \cdot I^{U} II^{V} III^{W} \cdot II_{\theta}^{S} III_{\theta}^{T} \cdot \boldsymbol{I}^{U'} \boldsymbol{II}^{V'} \boldsymbol{III}^{W'}\right]_{k(g)}, \quad \text{(V. 3)}$$

where q_0^{*} is the BOLTZMANN factor of the reversible work required to bring up the constituent particles of critical complex from their standard states to a definite, preliminarily unoccupied σ^{*} to compose the critical complex there, exclusive of the work due to interactions with surrounding hydrogen adatoms and expressed as[5],

$$q_0^{*} = \prod_{i=1}^{5} \left\{1-\exp(-h\nu_i^{*}/kT)\right\}^{-1} \cdot \exp\left(-\frac{\varepsilon_g^{*}}{RT}\right), \quad \text{(V. 4)}$$

where ε_g^{*} is the energy of the critical complex in the ground state. U', V' or W' is the number of adatoms inside $\sum$, which exert on the critical complex the repulsion of potential R_{I}^{*}, R_{II}^{*} or R_{III}^{*} respectively.

The $\Omega C^{*}_{\sigma^{*}(*)}$ of Eq. (V.3) is now worked out for all possible arrangements of hydrogen adatoms of all possible numbers inside $\sum$, as shown in Table IV in the Appendix for (110)–, (100)– and (111)–lattice planes, where $G=4$, $M=N=U=W=V'=W'=0$ for (110)–, $G=6$, $L=W=T=W'=0$ for (100)– and $G=8$, $L=V=S=0$ for (111)–lattice planes. Eq. (V.3) is written rearranging the terms shown in Table IV as below.

(110)–lattice plane:

$$\Omega C^{*}_{\sigma^{*}(*)} = \Omega C_{\Sigma(0)} \cdot q_0^{*}\zeta^{*} \cdot \mathrm{SUM}(110)^{*}, \quad \mathrm{SUM}(110)^{*} \equiv \sum_{j=1}^{5} d_{1,j} X^{j-1}, \quad \text{(V. 5. a)}$$

(100)–lattice plane:

$$\Omega C^{*}_{\sigma^{*}(*)} = \Omega C_{\Sigma(0)} \cdot q_0^{*}\zeta^{*} \cdot \mathrm{SUM}(100)^{*}, \quad \text{(V. 5. b)}$$

$$\mathrm{SUM}(100)^{*} \equiv \sum_{j=1}^{5} (d_{1,j} + d_{2,j}Z + d_{3,j}Z^{2}) Y^{j-1},$$

(111)–lattice plane:

$$\Omega C^{*}_{\sigma^{*}(*)} = \Omega C_{\Sigma(0)} \cdot q_0^{*}\zeta^{*} \cdot \mathrm{SUM}(111)^{*},$$

TABLE 16. Constants $d_{k,j}$ in Eqs. (V.5.a) and (V.7.a) for (110)–lattice plane.

k \ j	1	2	3	4	5
1	1	$4\boldsymbol{I}$	$4\boldsymbol{I}^{2}+2II\,\boldsymbol{I}^{2}$	$4II\,\boldsymbol{I}^{3}$	$II^{2}\boldsymbol{I}^{4}$
2	1	4	$4+2II$	$4II$	II^{2}
3	2	$4I+4III$	$2I^{2}+4I\,II\,III+4I\,III+2III^{2}$	$4I^{2}II\,III+4I\,II\,III^{2}$	$2I^{2}II^{2}III^{2}$
4	II	$4I\,II\,III$	$4I^{2}II\,III^{2}+2I^{2}II^{2}III^{2}$	$4I^{3}II^{2}III^{3}$	$I^{4}II^{3}III^{4}$

TABLE 17. Constants, $d_{k,j}$ in Eqs. (V.5.b) and (V.7.b) for (100)-lattice plane.

k \ j	1	2	3	4	5
1	1	$4\boldsymbol{II}$	$4\boldsymbol{II}^2+2I\,\boldsymbol{II}^2$	$4I\,\boldsymbol{II}^3$	$I^2\,\boldsymbol{II}^4$
2	$2\boldsymbol{I}$	$4\boldsymbol{I}\,\boldsymbol{II}+4II\,\boldsymbol{I}\,\boldsymbol{II}$	$2\boldsymbol{I}\,\boldsymbol{II}^2+4II\,\boldsymbol{I}\,\boldsymbol{II}^2$ $+2II^2\,\boldsymbol{I}\,\boldsymbol{II}^2+4I\,II\,\boldsymbol{I}\,\boldsymbol{II}^2$	$4I\,II\,\boldsymbol{I}\,\boldsymbol{II}^3$ $+4I\,II^2\,\boldsymbol{I}\,\boldsymbol{II}^3$	$2I^2II^2\,\boldsymbol{I}\,\boldsymbol{II}^4$
3	$\boldsymbol{I}^2$	$4II\,\boldsymbol{I}^2\,\boldsymbol{II}$	$4II^2\,\boldsymbol{I}^2\boldsymbol{II}^2+2I\,II^2\,\boldsymbol{I}^2\boldsymbol{II}^2$	$4I\,II^3\,\boldsymbol{I}^2\boldsymbol{II}^3$	$I^2II^4\,\boldsymbol{I}^2\boldsymbol{II}^4$
4	1	4	$4+2I$	$4I$	I^2
5	2	$4+4II$	$2+4II+2II^2+4I\,II$	$4I\,II+4I\,II^2$	$2I^2II^2$
6	1	$4II$	$4II^2+2I\,II^2$	$4I\,II^3$	I^2II^4
7	2	$4II+4I$	$2II^2+4I\,II+2I^2+4I^2II$	$4I^2II^2+4I^3II$	$2I^4II^2$
8	I	$4I^2II$	$4I^3II^2+2I^4II^2$	$4I^5II^3$	I^7II^4
9	$2+2I$	$4II^2+4I+4I\,II$ $4I^2II$	$2II^4+6I\,II^2+2I^2+8I^2II^2$ $+2I^3II^2$	$4I^2II^4+4I^3II^2$ $+4I^3II^3+4I^4II^3$	$2I^4II^4$ $+2I^5II^4$
10	$2I^2$	$4I^3II+4I^3II^2$	$2I^4II^2+4I^4II^3+2I^4II^4$ $+4I^5II^3$	$4I^6II^4+4I^6II^5$	$2I^8II^6$
11	$2I$	$4I\,II^2+4I^2II$	$2I\,II^4+4I^2II^3+2I^3II^2$ $+4I^3II^3$	$4I^3II^5+4I^4II^4$	$2I^5II^6$
12	I^3	$4I^4II^2$	$4I^5II^4+2I^6II^4$	$4I^7II^6$	I^9II^8

$$\mathrm{SUM}\,(111)^{*}=\sum_{j=1}^{7}(d_{1,j}+d_{2,j}Z+d_{3,j}Z^2)\,Y^{j-1}\,, \qquad \text{(V. 5. c)}$$

and $d_{k,j}$'s are constants shown in Tables 16, 17 and 18 for the respective lattice planes.

$\mathfrak{Q}C$: $\mathfrak{Q}C$ is expressed with reference to $\sum$ on each lattice plane as the sum of $\mathfrak{Q}C_{\sigma_{\hat{\imath}}(\mathrm{H})}$ and $\mathfrak{Q}C_{\sigma_{\hat{\imath}}(0)}$ worked out in §4-1, as

$$\begin{aligned}\mathfrak{Q}C&=\sum_{g=0}^{G}\sum_{k(g)=1}^{K(g)}\mathfrak{Q}C_{\sum(G\sigma(g\,\mathrm{H})_{k(g)}}\\&=\sum_{g=0}^{G}\sum_{k\,(g)=1}^{K(g)}\mathfrak{Q}C_{\sum(0)}\cdot\gamma^{g}\cdot\left[\rho_1^{L}\rho_2^{M}\rho_3^{N}\cdot I^{U}II^{V}III^{W}\cdot II_{\theta}^{S}III_{\theta}^{T}\right]_{k(g)}\,.\end{aligned} \qquad \text{(V. 6)}$$

We have here no specification for the state of σ's in $\sum$, *e.g.* that a definite

TABLE 18. Constants, $d_{k,j}$ in Eqs. (V.5.c) and (V.7.c) for (111)–lattice plane.

k \ j	1	2	3	4	5	6	7
1	1	$2\boldsymbol{I}+4\boldsymbol{II}$	$4I\,\boldsymbol{I\,II}+4\boldsymbol{I\,II}+\boldsymbol{I}^2$ $+4\boldsymbol{II}^2+2III\,\boldsymbol{II}^2$	$8\boldsymbol{I\,I\,II}^2+4\boldsymbol{I}^2\boldsymbol{II}$ $+2I^2III\,\boldsymbol{I\,II}^2$ $+2III\,\boldsymbol{I\,II}^2+4III\,\boldsymbol{II}^3$	$4I^2\,\boldsymbol{I}^2\boldsymbol{II}^2+4I\,III\,\boldsymbol{I\,II}^3$ $+4I^2III\,\boldsymbol{I\,II}^3$ $+2I^2III\,\boldsymbol{I}^2\boldsymbol{II}^2+III^2\boldsymbol{II}^4$	$4I^3III\,\boldsymbol{I}^2\boldsymbol{II}^3$ $+2I^2III^3\,\boldsymbol{I\,II}^4$	$I^4III^2\,\boldsymbol{I}^2\boldsymbol{II}^4$
2	$2\boldsymbol{III}$	$4III\,\boldsymbol{I\,III}$ $+4I\,\boldsymbol{II\,III}$ $+4\boldsymbol{II\,III}$	$4I^2III\,\boldsymbol{I\,II\,III}$ $+8I\,III\,\boldsymbol{I\,II\,III}$ $+2III^2\boldsymbol{I}^2\boldsymbol{III}$ $+4III\,\boldsymbol{I\,II\,III}$ $+2I^2\,\boldsymbol{II}^2\boldsymbol{III}$ $+4I\,\boldsymbol{II}^2\boldsymbol{III}$ $4I\,III\,\boldsymbol{II}^2\boldsymbol{III}$ $+2\boldsymbol{II}^2\boldsymbol{III}$	$4I^3III\,\boldsymbol{I\,II}^2\boldsymbol{III}$ $+4I^2III^2\,\boldsymbol{I}^2\boldsymbol{II\,III}$ $+8I^2III\,\boldsymbol{I\,II}^2\boldsymbol{III}$ $+4I^3III^2\,\boldsymbol{I\,II}^2\boldsymbol{III}$ $+4I\,III\,\boldsymbol{I\,II}^2\boldsymbol{III}$ $+4I\,III^2\,\boldsymbol{I\,II}^2\boldsymbol{III}$ $+4I^2III\,\boldsymbol{II}^3\boldsymbol{III}$ $+4I\,III\,\boldsymbol{II}^3\boldsymbol{III}$ $+4I\,III^2\,\boldsymbol{I\,II}^2\boldsymbol{III}$	$2I^4III^2\,\boldsymbol{I}^2\boldsymbol{II}^2\boldsymbol{III}$ $+8I^3III^2\,\boldsymbol{I\,II}^3\boldsymbol{III}$ $+4I^4III^2\,\boldsymbol{I\,II}^3\boldsymbol{III}$ $+4I^3III^2\,\boldsymbol{I}^2\boldsymbol{II}^2\boldsymbol{III}$ $+4I^3III^3\,\boldsymbol{I}^2\boldsymbol{II}^2\boldsymbol{III}$ $+2I^2III^2\,\boldsymbol{I}^2\boldsymbol{II}^2\boldsymbol{III}$ $+4I^2III^2\,\boldsymbol{I}^2\boldsymbol{II}^3\boldsymbol{III}$ $+2I^2III^2\,\boldsymbol{II}^4\boldsymbol{III}$	$4I^5III^3\,\boldsymbol{I}^2\boldsymbol{II}^3\boldsymbol{III}$ $+4I^4III^3\,\boldsymbol{I\,II}^4\boldsymbol{III}$ $+4I^4III^3\,\boldsymbol{I}^2\boldsymbol{II}^3\boldsymbol{III}$	$2I^6III^4\,\boldsymbol{I}^2\boldsymbol{II}^4\boldsymbol{III}$
3	$III\,\boldsymbol{III}^2$	$2III^3\,\boldsymbol{I\,III}^2$ $+4I\,III\,\boldsymbol{II\,III}^2$	$4I^2III^3\,\boldsymbol{I\,II\,III}^2$ $+4I\,III^3\,\boldsymbol{I\,II\,III}^2$ $+III^5\boldsymbol{I}^2\boldsymbol{III}^2$ $+4I^2III\,\boldsymbol{II}^2\boldsymbol{III}^2$ $+2I^2III^2\,\boldsymbol{II}^2\boldsymbol{III}^2$	$8I^3III^3\,\boldsymbol{I\,II}^2\boldsymbol{III}^2$ $+4I^2III^5\,\boldsymbol{I}^2\boldsymbol{II\,III}^2$ $+2I^4III^4\,\boldsymbol{I\,II}^2\boldsymbol{III}^2$ $+2I^2III^4\,\boldsymbol{I\,II}^2\boldsymbol{III}^2$ $+4I^3III^2\,\boldsymbol{II}^2\boldsymbol{III}^2$	$4I^4III^5\,\boldsymbol{I}^2\boldsymbol{II}^2\boldsymbol{III}^2$ $+4I^4III^4\,\boldsymbol{I\,II}^3\boldsymbol{III}^2$ $+4I^5III^4\,\boldsymbol{I\,II}^3\boldsymbol{III}^2$ $+2I^4III^6\,\boldsymbol{I}^2\boldsymbol{II}^3\boldsymbol{III}^2$ $+I^4III^3\,\boldsymbol{II}^4\boldsymbol{III}^2$	$4I^6III^6\,\boldsymbol{I}^2\boldsymbol{II}^3\boldsymbol{III}^2$ $+2I^6III^5\,\boldsymbol{I\,II}^4\boldsymbol{III}^2$	$I^8III^7\boldsymbol{I}^2\boldsymbol{II}^4\boldsymbol{III}^2$
4	1	6	$9+2III+4I$	$6III+12I+2I^2III$	$III^2+4I\,III+4I^2$ $+6I^2III$	$2I^2III^2+4I^3III$	I^4III^2
5	2	$4+4III+4I$	$2+4III+2III^2+4I$ $+12I\,III+2I^2$ $+4I^2III$	$8I\,III+8I\,III^2+12I^2III$ $+4I^3III+4I^3III^2$	$8I^2III^2+12I^3III^2$ $+4I^3III^3+6I^4III^2$	$8I^4III^3+4I^5III^3$	$2I^6III^4$
6	III	$2III^3+4I\,III$	$III^5+4I\,III^3$ $+4I^2III+2I^2III^2$ $+4I^2III^3$	$2I^2III^4+4I^2III^5$ $+4I^3III^2+8I^3III^3$ $+2I^4III^4$	$I^4III^3+4I^4III^4$ $+4I^4III^5+2I^4III^6$ $+4I^5III^4$	$2I^6III^5+4I^6III^6$	I^8III^7
7	2	$2+4III+6I$	$2III^3+6I+16I\,III$ $+2I^2III+4I^3$	$6I\,III^3+14I^2III$ $+4I^2III^2+2I^2III^3$ $+4I^3+8I^3III+2I^5III$	$2I^2III^2+4I^3III^2$ $+10I^3III^3+8I^4III$ $+2I^5III+4I^5III^2$	$2I^4III^4+4I^5III^3$ $+2I^5III^4+4I^6III^2$	$2I^7III^4$
8	I	$2I^2+4I^2III$	$I^3+4I^3III+4I^3III^2$ $+2I^3III^3+4I^4III$	$2I^4III^3+4I^4III^4$ $+4I^5III+8I^5III^2$ $+2I^6III^3$	$I^5III^6+4I^6III^4$ $+4I^7III^2+2I^7III^3$ $+4I^7III^4$	$2I^8III^6+4I^9III^4$	$I^{11}III^6$
9	$4I$	$8I\,III+4I^2$ $+8I^2III+4I^3$	$8I^2III+12I^2III^2$ $+4I^2III^3+12I^3III$ $+8I^3III^2+12I^4III$ $+4I^5III$	$4I^3III^2+8I^3III^3$ $+4I^3III^4+24I^4III^2$ $+8I^4III^3+4I^4III^4$ $+20I^5III^2+4I^6III^2$ $+4I^7III^2$	$8I^5III^3+12I^5III^4$ $+4I^5III^6+12I^6III^3$ $+8I^6III^4+12I^7III^3$ $+4I^8III^3$	$8I^7III^5+4I^8III^4$ $+8I^8III^5+4I^9III^4$	$4I^{10}III^6$
10	$2I^3$	$8I^4III+4I^5III$	$8I^5III^2+12I^6III^2$ $+4I^6III^3+6I^7III^2$	$8I^7III^3+8I^7III^4$ $+12I^8III^3+4I^8III^4$ $+4I^9III^3+4I^9III^4$	$2I^9III^4+4I^9III^5$ $+2I^9III^6+4I^{10}III^4$ $+12I^{10}III^5+2I^{11}III^4$ $+4I^{11}III^5$	$4I^{12}III^6+4I^{12}III^7$ $+4I^{13}III^6$	$2I^{15}III^8$
11	$2I^2III$	$2I^2III^3+4I^3III^2$ $+2I^3III^3+4I^4III$	$2I^2III^5+4I^4III^3$ $+10I^4III^4+8I^5III^2$ $+2I^6III^2+4I^6III^3$	$6I^5III^6+14I^6III^4$ $+4I^6III^5+2I^6III^6$ $+4I^7III^3+8I^7III^4$ $+2I^9III^4$	$2I^7III^8+6I^8III^5$ $+16I^8III^6+2I^9III^6$ $+4I^{10}III^5$	$2I^{10}III^7+4I^{10}III^8$ $+6I^{11}III^7$	$2I^{13}III^9$
12	I^5III	$2I^6III^3+4I^7III^2$	$I^7III^5+4I^8III^4$ $+4I^9III^3+6I^9III^4$	$6I^{10}III^6+12I^{11}III^5$ $+2I^{12}III^6$	$9I^{13}III^7+2I^{12}III^8$ $+4I^{14}III^7$	$6I^{16}III^9$	$I^{19}III^{11}$

pair of σ's are occupied by the critical complex, hence $G=6$, $M=N=0$ for (110)–, $G=8$, $L=W=T=0$ for (100)– or $G=10$, $L=V=S=0$ for (111)–lattice plane respectively; all terms of the sums in Eq. (V.6) are shown in Table V in the Appendix. The terms thus obtained are rearranged as below.

(110)–lattice plane:

$$\Omega C = \Omega C_{\Sigma(0)}\,\mathrm{SUM}(110),$$

$$\mathrm{SUM}(110) = \sum_{j=1}^{5}(d_{2,j}+d_{3,j}\zeta+d_{4,j}\zeta^2)X^{j-1}, \qquad \text{(V. 7. a)}$$

(100)–lattice plane:

$$\Omega C = \Omega C_{\Sigma(0)}\,\mathrm{SUM}(100),$$

$$\mathrm{SUM}(100) = \sum_{j=1}^{5}(d_{4,j}+d_{5,j}Z+d_{6,j}Z^2+d_{7,j}\zeta+d_{8,j}\zeta^2+d_{9,j}\zeta Z+ +d_{10,j}\zeta^2 Z+d_{11,j}\zeta Z^2+d_{12,j}\zeta^2Z^2)Y^{j-1}, \qquad \text{(V. 7. b)}$$

(111)–lattice plane:

$$\Omega C = \Omega C_{\Sigma(0)}\,\mathrm{SUM}(111),$$

$$\mathrm{SUM}(111) = \sum_{j=1}^{7}(d_{4,j}+d_{5,j}Z+d_{6,j}Z^2+d_{7,j}\zeta+d_{8,j}\zeta^2+d_{9,j}\zeta Z+ +d_{10,j}\zeta^2 Z+d_{11,j}\zeta Z^2+d_{12,j}\zeta^2Z^2)Y^{j-1}, \qquad \text{(V. 7. c)}$$

where $d_{k,j}$'s are constants shown in Tables 16, 17 and 18 for the respective lattice planes.

It follows from Eqs. (V.5) and (V.7) that $\Omega C^*_{\sigma^*(*)}/\Omega C$ is reduced to $q_0^*\zeta^*\cdot \mathrm{SUM}(110)^*/\mathrm{SUM}(110)$, $q_0^*\zeta^*\ \mathrm{SUM}(100)^*/\mathrm{SUM}(100)$ and $q_0^*\zeta^*\ \mathrm{SUM}(111)^*/\mathrm{SUM}(111)$ in the respective cases of the lattice planes, $\Omega C_{\Sigma(0)}$ being cancelled out, where q_0^* is the factor independent of η as seen from Eq. (V.4). $\Omega C^*_{\sigma^*(*)}/\Omega C$ is now evaluated as a function of η according to the above equations using numerical values of X, Y, Z and θ given in Tables 14 and 15.

The latter quantities especially X, Y or Z which comprizes ρ_1, ρ_2 or ρ_3 have had to be evaluated with special reference to the $\sum$ employed in the respective case of the lattice plane.

The $\Omega C^*_{\sigma^*(*)}/\Omega C$ is calculated by the proportional approximation as well, for the (110)–lattice plane for comparison. The $\sum$ is reduced in this case to σ^* as mentioned in §4–3, hence we have

$$\Omega C^*_{\sigma^*(*)} = \Omega C_{\sigma^*(0)} q_0^*\zeta^* \qquad \text{(V. 8)}$$

and from Eqs. (IV.1), (IV.31.a) and (IV.31.b)

$$\mathfrak{Q}C = \mathfrak{Q}C_{\sigma^*(0)}(1+2\gamma\cdot I_\theta^2 II_\theta III_\theta^4+\gamma^2\cdot II\cdot I_\theta^4 II_\theta^2 III_\theta^8)\,, \qquad (V.9)^{*)}$$

where $-RT\ln\zeta^*=(4R_{\mathrm{I}}^*+2R_{\mathrm{II}}^*+4R_{\mathrm{III}}^*)\theta$ as seen from Fig. 5. The above two equations are reduced in the absence of interaction, *i.e.* for $\alpha=0$, where $I_\theta=II_\theta=III_\theta=\zeta^*=1$, to the equations

$$\mathfrak{Q}C_{\sigma^*(*)}^* = \mathfrak{Q}C_{\sigma^*(0)}\cdot q_0^* \qquad (V.10)$$

$$\mathfrak{Q}C = \mathfrak{Q}C_{\sigma^*(0)}(1+\gamma)^2\,. \qquad (V.11)$$

We have from Eqs. (V.8) to (V.11) in case of the proportional approximation,

$$\mathfrak{Q}C_{\sigma^*(*)}^*/\mathfrak{Q}C = q_0^*\zeta^*/(1+2\gamma\cdot I_\theta^2 II_\theta III_\theta^4+\gamma^2\cdot II\cdot I_\theta^4 II_\theta^2 III_\theta^8)\,, \qquad (V.12)$$

which is reduced for $\alpha=0$ to the equation

$$\mathfrak{Q}C_{\sigma^*(*)}^*/\mathfrak{Q}C = q_0^*/(1+\gamma)^2\,. \qquad (V.13)$$

§ 5–3. Current Densities

Final expression of the current density is now given according to Eqs. (I.7.i_+), (V.5) and (V.7) as

$$i_+ = 2e^-\frac{kT}{h}N^{\mathrm{H}_2}\cdot N_1^*\cdot\frac{q_0^*}{Q^{\mathrm{H}_2}}\cdot\Gamma\cdot\exp\left(\frac{2F\eta}{RT}\right), \qquad (V.14)$$

where $\Gamma\equiv\zeta^*$ SUM (110)*/SUM (110), ζ^* SUM (100)*/SUM (100) or ζ^* SUM (111)*/SUM (111) for (110)–, (100)– or (111)–lattice plane respectively. The first factor $2e^-(kT/h)N^{\mathrm{H}_2}$ on the right side of Eq. (V.14) is common to all expressions of i_+ on the different lattice planes. The second factor N_1^* depends on the lattice plane as

$$N_1^* = 1\times10^{15}\,,\quad 3\times10^{15}\quad\text{or}\quad 6\times10^{15}\ \mathrm{cm}^{-2} \qquad (V.15.N)$$

respectively for the (110)–, (100)– or (111)–lattice plane. The third factor q_0^*/Q^{H_2} is expressed by Eqs. (I.5.Q^{H_2}) and (V.4) as

$$\frac{q_0^*}{Q^{\mathrm{H}_2}} = \frac{\prod_{i=1}^{5}\left\{1-\exp\left(-\frac{h\nu_i^*}{kT}\right)\right\}^{-1}}{(2\pi mkT)^{3/2}\,4\pi^2 IkT/h^5}\cdot\exp\left(-\frac{\varepsilon_{g_0}^*-\varepsilon_g^{\mathrm{H}_2}}{RT}\right).$$

*) The previous formulation[7] $\theta^*(0)=(1-\theta)(1-\theta')$ of the probability $\theta^*(0)$ of seat σ^* of the critical complex being unoccupied, is erroneous, where θ is the probability of one of the constituent sites of σ^* being occupied irrespective as to whether the second site of σ^* is occupied or not and θ' the probability of the second site being occupied in case, where the first site is unoccupied. The probability of the first site being unoccupied depends reciprocally upon whether the second site is occupied or not, insofar as that of the second site does upon whether the first site is occupied or not. The probability that the first site is unoccupied should in consequence differ from the first factor $(1-\theta)$ in case, where the second site is unoccupied and there exists interaction, hence $(1-\theta)(1-\theta')$ does not equal $\theta^*(0)$.

TABLE 19. Theoretical values of $\log i_+$ (A cm^{-2}) on (110)-, (100)-

Combined Approximation

(110)				(100)				(111)	
$\eta/59.1$	$\alpha=1.2$	$\alpha=1.5$	$\alpha=2.5$	$\eta/59.1$	$\alpha=1.2$	$\alpha=1.5$	$\alpha=2.5$	$\eta/59.1$	$\alpha=1.2$
−9.51	−16.37	−16.37	−16.37	−6.56	−15.96	−15.96	−15.96	−4.71	−12.17
−8.51	−14.44	−14.44	−14.44	−5.56	−14.06	−14.06	−14.07	−3.71	−10.28
−7.51	−12.86	−12.86	−12.83	−4.56	−12.54	−12.55	−12.57	−2.71	−8.79
−6.51	−11.96	−11.94	−11.82	−3.56	−11.58	−11.58	−11.57	−1.71	−7.76
−5.51	−11.51	−11.53	−11.36	−2.56	−11.00	−11.00	−10.92	−0.71	−6.88
−4.51	−11.04	−11.23	−11.19	−1.56	−10.59	−10.60	−10.53	0.29	−5.97
−3.51	−10.30	−10.74	−11.11	−0.56	−10.27	−10.26	−10.21	1.29	−5.03
−2.51	−9.30	−9.92	−10.98	0.44	−9.83	−10.13	−9.84	2.29	−4.07
−1.51	−8.44	−8.81	−10.68	1.44	−9.15	−9.76	−9.48	3.29	−3.09
−0.51	−8.10	−7.79	−10.07	2.44	−8.28	−9.11	−9.31	4.29	−2.21
0.49	−8.04	−7.30	−9.09	3.44	−7.42	−8.28	−9.07	5.29	−1.75
1.49	−8.04	−7.21	−7.77	4.44	−6.82	−7.26	−8.87	6.29	−1.38
2.49	−8.04	−7.19	−6.31	5.44	−6.47	−6.33	−8.66	7.29	−0.94
3.49	−8.04	−7.19	−5.13	6.44	−6.28	−5.70	−8.43	8.29	−0.47
4.49	−8.04	−7.19		7.44	−6.24	−5.43	−7.85	9.29	−0.14
5.49	−8.04	−7.19		8.44	−6.24		−6.94	10.29	−0.13
				9.44			−5.74	11.29	−0.70
				10.44			−4.45	12.29	−1.99
				11.44			−3.27	13.29	
				12.44			−2.36	14.29	
				13.44			−1.75	15.29	
				14.44			−1.44	16.29	
				15.44			−1.23	17.29	
				16.44			−1.11	18.29	
				17.44			−1.08	19.29	
				18.44			−1.08	20.29	
				19.44			−1.08	21.29	
				20.44			−1.08	22.29	
				21.44			−1.08	23.29	
								24.29	
								25.29	

and (111)-lattice planes at 25°C and 1 atm pressure of hydrogen.

		Proportional Approximation					No Interaction	
(111)		(110)					(110)	
$\alpha=1.5$	$\alpha=2.5$	$\eta/59.1$	$\alpha=1.0$	$\alpha=1.5$	$\alpha=2.0$	$\alpha=2.5$	$\alpha=4.4$	$\eta/59.1$	$\alpha=0$
−12.17	−12.17	−9.51	−16.38	−16.39	−16.40	−16.40	−16.39	−9.51	−16.36
−10.29	−10.30	−7.51	−13.01	−13.10	−13.18	−13.25	−13.41	−8.51	−14.39
−8.81	−8.84	−5.51	−10.92	−11.06	−11.13	−11.21	−11.39	−8.01	−13.45
−7.82	−7.90	−3.51	−9.38	−9.34	−9.41	−9.50	−9.64	−7.71	−12.93
−7.00	−7.20	−2.51	−8.87					−7.51	−12.61
−6.17	−6.58	−1.51	−8.54	−7.91	−7.81	−7.85	−7.99	−7.31	−12.33
−5.28	−5.94	−0.51	−8.45	−7.40				−7.11	−12.09
−4.32	−5.05	0.49		−7.09	−6.44	−6.29	−6.40	−6.91	−11.90
−3.34	−4.35	1.49		−6.97	−5.96			−6.71	−11.75
−2.29	−3.43	2.49			−5.64	−4.95	−4.86	−6.51	−11.64
−1.21	−2.45	3.49			−5.50	−4.50		−6.31	−11.56
−0.48	−1.43	4.49				−4.16	−3.39	−6.11	−11.51
−0.16	−0.37	5.49				−4.02		−5.91	−11.47
0.16	0.76	6.49					−1.99	−5.71	−11.45
0.59	1.99	8.49					−0.65	−5.51	−11.43
1.18	3.30	10.49					0.58	−5.31	−11.43
1.64	4.32	12.49					1.49	−5.11	−11.42
2.00	4.61	13.49					1.66	−4.91	−11.42
2.07	4.77							−4.71	−11.41
1.62	4.96								
0.32	5.27								
−1.27	5.64								
−2.18	6.10								
−2.37	6.61								
−2.39	7.45								
−2.39	7.87								
−2.39	8.78								
	8.91								
	9.35								
	8.97								
	8.44								

The value of $\varepsilon_g^* - \varepsilon_g^{H_2}$ was determined in accordance with the conclusion of the previous work[7] as derived from the experimental results[8], that the activation energy of hydrogen adsorption on Ni is zero at the very initial stage at room temperature, where interaction is ignorable; the rate v_- of the dissociative adsorption is given by v_+ of Eq. (I.1) by substituting p^{H_2} from Eq. (I.4.H_2) for p^I and p^* there from Eq. (I.6), inasmuch as H_2 is the initial system I in this case; since $\Omega C^*_{\sigma^*(*)}/\Omega C$ is reduced in the latter extreme condition to q_0^*

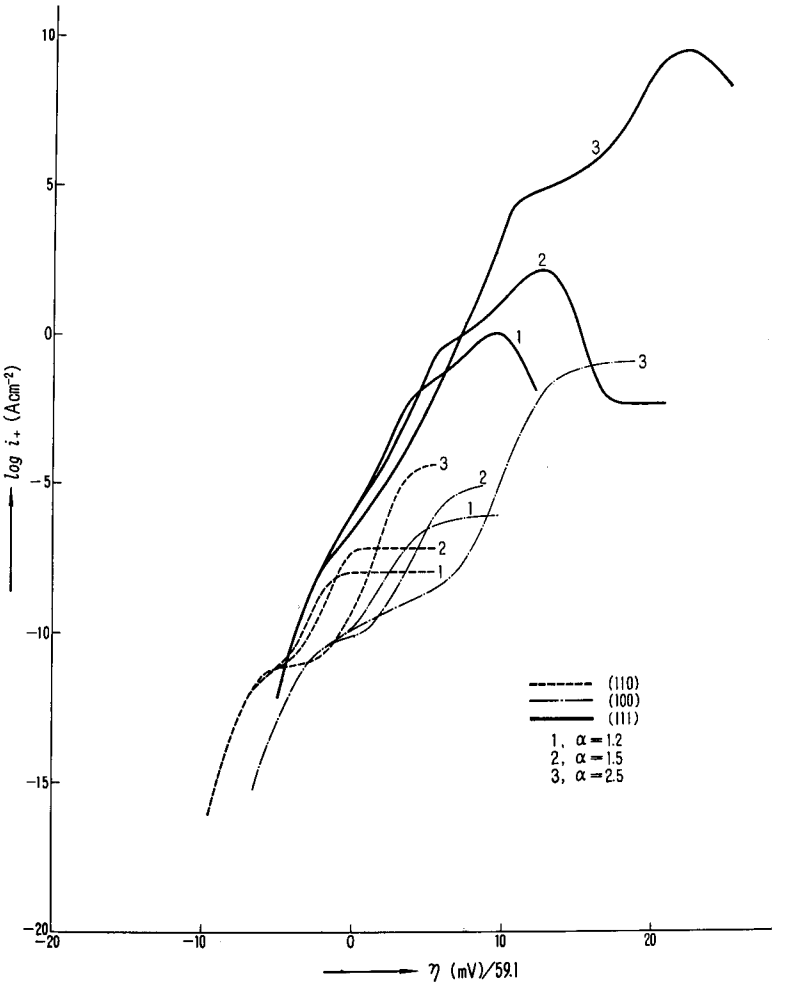

Fig. 10. Theoretical $\log i_+ \sim \eta$ relation of hydrogen evolution reaction on (110)-, (100)- and (111)-lattice planes of Ni obtained by the combined approximation for $\alpha = 1.2$, 1.5 and 2.5 at 25°C and 1 atm pressure of hydrogen.

according to Eq. (V.13) with reference to Eq. (IV.33), we have[7]

$$v_- = (kT/h)N^{H_2}N_1^{*}q_0^{*}/Q^{H_2}, \quad \text{hence}$$

$$RT^2\left(\frac{\partial \log v_-}{\partial T}\right)_{\mu^{H_2}} = 0 = \varepsilon_g^{*} - RT^2\frac{d\log Q^{H_2}}{dT} = \varepsilon_g^{*} - \varepsilon_g^{H_2} - 5/2\cdot RT,$$

identifying q_0^{*} approximately with $\exp(-\varepsilon_g^{*}/RT)$, where P^{H_2} is the pressure of hydrogen gas kept constant, or

$$\varepsilon_g^{*} - \varepsilon_g^{H_2} = 5/2\cdot RT \qquad (V.15.\ \varepsilon_g^{*})$$

for (110)-lattice plane, admitting that adsorption occurs predominantly on the (110)-lattice plane at its very initial stage.*) The values of $\varepsilon_g^{*} - \varepsilon_g^{H_2}$ on the other lattice planes are determined by adding the appropriate difference of $\varepsilon'^{*} + \sum_j (K_j - 1/2\cdot J_j)$ given in Table 3 to $5RT/2$. The values of ν^{*} are shown in Table 4 and those of m and I are taken as $2.016/6.024\times 10^{23}$ and 4.664×10^{-41} g cm.^{2}[21] Using Eqs. (V.14) and (V.15) as well as values of Γ's calculated in §5-2, i_+ on the respective planes are determined at 25°C, 1 atm pressure of hydrogen, assuming that each lattice plane is developed equally by one third of the total area. The results are shown in Table 19 and Fig. 10.

Fig. 10 shows that the slope of $\log i_+$ against η is $2F/2.303RT$, *i.e.* $\tau=2$ at very low current densities. With increase of current density, however, the slope changes in a complicated manner and tends finally to zero, *i.e.* $\tau=0$ as seen in Fig. 10 or readily deduced, revealing the saturation current.

Fig. 11 shows $\log i_+ \sim \eta$ plots on each lattice plane for $\alpha=1.5$ in comparison with the experimental results[22] as well as with the theoretical calculations on (110)-lattice plane by the proportional approximation for $\alpha=0$ and 4.4 respectively.

The following points are remarked with regard to Fig. 11.

(**1**) The saturation current density at $\eta\to\infty$ increases in the order of (110)-, (100)- and (111)-lattice planes. The (111)-lattice plane contributes predominantly to the current density at overvoltage above 0.2 V, where observations of i_+ are usually practiced as mentioned in §4-4.

(**2**) Log $i_+\sim\eta$ plot deviates without taking repulsive interactions into account, *i.e.* for $\alpha=0$, far from the observed one, indicating the important part played by the repulsion between unbonded hydrogen atoms, as deduced quantum-mechanically to exist.[12]

(**3**) The $\log i_+\sim\eta$ relation calculated by the proportional approximation for $\alpha=4.4$ on the basis of the (110)-lattice plane is in fair agreement with

*) It is seen from Fig. 8a that the hydrogen adsorption occurs predominantly on the (110)-lattice plane at the very low activity of hydrogen adatom or such overvoltage.

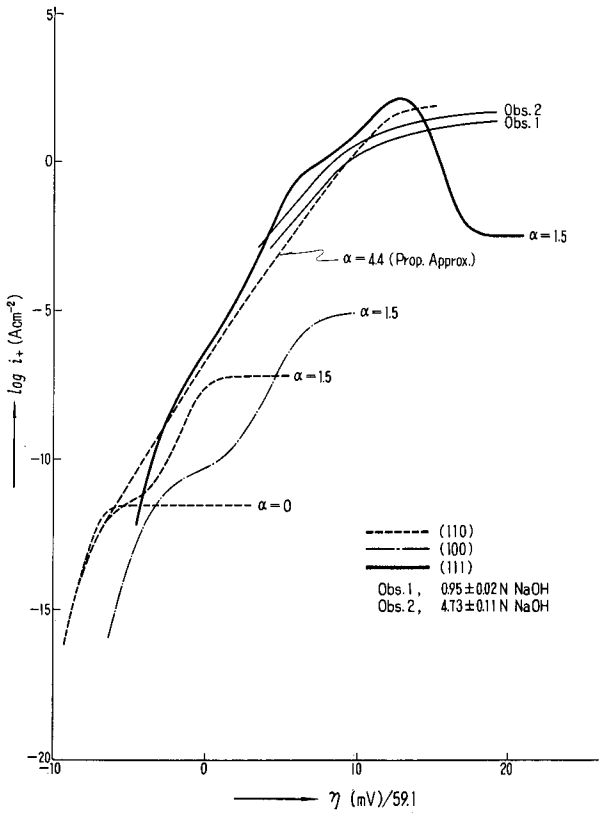

Fig. 11. Comparison of the experimental $\log i_+ \sim \eta$ relation with the theoretical ones by the combined approximation for $\alpha = 1.5$ on (110)-, (100)- and (111)-lattice planes of Ni as well as by the proportional approximation for $\alpha = 0$ and 4.4 on (110)-lattice plane.

the observed one, giving constant slope of $\tau = 0.65$, whereas this value of α is far too large as compared with the value 1.5 determined from the analysis of adsorption isotherms[11], for such low activity of hydrogen adatoms as the adsorption occurs predominantly on (110)-lattice plane. The present investigation shows now that the predominant contribution to the rate is due to the (111)-lattice plane over the range of η, where the i_+ is usually observed. The above discrepancy of α-value is reconciled reasonably by transferring from the (110)-to (111)-lattice plane with the proportional approximation, inasmuch as the repulsive potential of an adatom is thus approximately trebled, since its first nearest neighbours contributing predominantly to the repulsive potential increases thus from 2 to 6, which is nearly equivalent to increasing α from

1.5 to 4.4 remaining instead with the (110)-lattice plane.

(**4**) $\mathrm{Log}\, i_+ \sim \eta$ relation on the (111)-lattice plane is quite different from others at higher current densities, where further increase of η is associated with a conspicuous decrease of current density, hence $\tau < 0$. This decrease of i_+ with increase of η is attributed to the repulsive potential, R^*_{III}, *i. e.* that between the hydrogen adatom on σ_5 or σ_9 in $\sum$ of (111)-lattice plane in Fig. 7 and the critical complex situated on σ_1 and σ_2. The repulsive potential R^*_{III} is extraordinary large, hence the sites σ_5 and σ_9 tend to remain unoccupied until the coverage attains *ca.* 0.8. With further increase of η, however, these sites are occupied, resulting in a large increase of the potential energy of the critical complex, hence in a considerable decrease in i_+. On the other lattice planes R^*_{II} or R^*_{I} is almost equal or less than R_{I} while R^*_{III} is absent as seen from Eqs. (IV.5) and (V.2). It follows in the latter case that sites are nearly equally covered, no such sites being left unoccupied till an extremely high overvoltage as their occupants, once emerged, severely increase the potential of the critical complex and hence decrease the current density as in the case of (111)-lattice plane.

(**5**) The experimental results of i_+ is torelably reproduced by its theoretical value of i_+, which is practically exclusively sustained by (111)-lattice plane in the region of overvoltage from 0.2 to 0.7 V. At higher overvoltage than 0.7 V, however, the theoretical values of i_+ deviates considerably from the observed ones. This difference might be attributed to the galvanostatic method employed[22], where constant currents are imposed, hence only fraction of the current might possibly cause the hydrogen electrode reaction, the rest being spent on other electrode reaction, *e. g.* discharge of sodium ion, resulting in a large increase of the electrode potential. The $\log i_+ \sim \eta$ relation theoretically deduced at high overvoltage might be experimentally reproduced by potentiostatic measurements of steady currents in acid solution.

§ 5-4. TAFEL Constant

TAFEL constant τ is now readily calculated according to Eq. (V.1) as a function of η using the values of $\Omega C^*_{\sigma^*(*)}/\Omega C$ obtained in §5-2 by different approximations. Results obtained by the combined approximations are shown in Fig. 12.

The τ thus decreases from 2 to zero with increase of η. The present theoretical results indicate that the value 2 of τ elementarily deduced in the Introduction, reveals itself at extremely low coverage of the hydrogen adatoms, *i. e.* at the very large positive polarization against the reversible hydrogen electrode, whereas under the usual experimental conditions where

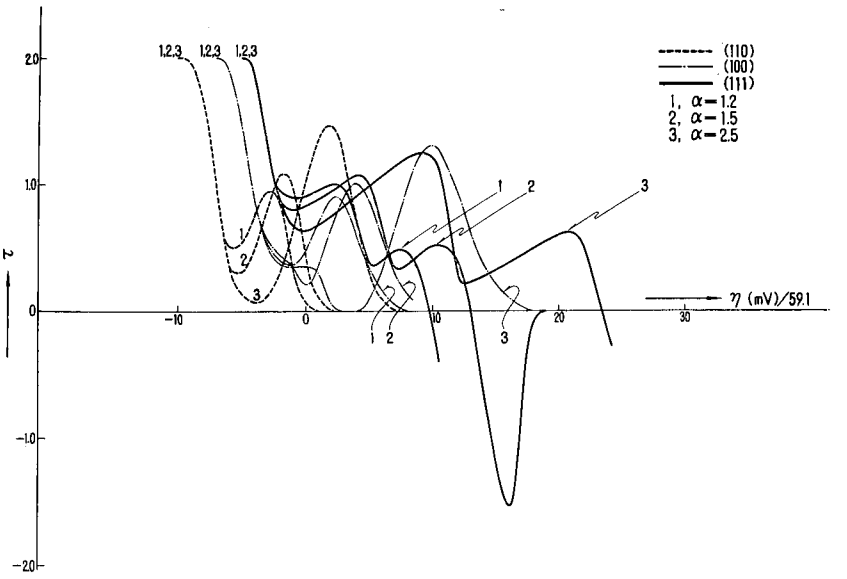

Fig. 12. Theoretical $\tau \sim \eta$ relation of hydrogen electrode reaction on (110)-, (100)- and (111)-lattice planes of Ni by the combined approximation for $\alpha = 1.2$, 1.5 and 2.5 at 25°C and 1 atm pressure of hydrogen.

$\eta > 0$*), the electrode surface is sufficiently covered with hydrogen atoms to reduce the value of τ from 2.

It is interesting to note that, in every cases studied by the combined approximation, τ reveals one or two maxima with increase of η, finally tending to zero at extremely high overvoltage. These behaviours are closely connected to those of θ (Fig. 8a) in such a way as the first or second minimum in $\tau \sim \eta$ diagram occurs at the value of overvoltage, where the first or second plateau appears in $\theta \sim \eta$ diagram. At the plateau, where θ increases with η only slightly, the increase of current density or τ with η is very small. As η increases above that of the plateau, θ and hence the current density increases rapidly with η, resulting in a rise of τ. As θ tends to its limiting value of unity, τ tends to zero. The $\tau \sim \eta$ plots for $\alpha = 1.5$ on the respective planes are compared with each other and with experimental values[22] as well as with those obtained by the proportional approximation for $\alpha = 0$ and 4.4 on (110)-lattice plane in Fig. 13.

Noting that the experiments are carried out in the overvoltage region higher than *ca.* 0.2 V, τ on (111)-lattice plane is in the best coincidence with

*) Overvoltage used in this paper is defined as negative of the potential of test electrode referred to that of the reversible hydrogen electrode in the same hydrogen atmosphere and the same electrolyte (*cf.* Introduction).

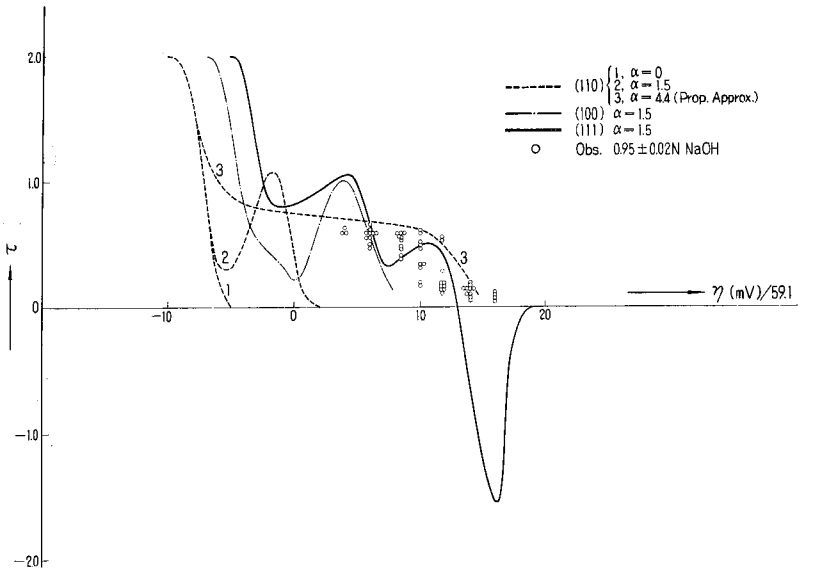

Fig. 13. Comparison of the experimental $\tau\sim\eta$ relation with the theoretical ones by the combined approximation for $\alpha=1.5$ on (110)–, (100)– and (111)–lattice planes of Ni as well as by the proportional approximation for $\alpha=0$ and 4.4 on the (110)–lattice plane.

the experimental results similarly to the case of $\log i_+\sim\eta$ plot, while τ's on the other planes are there almost reduced to zero, contributing practically none to the value of τ. The τ for $\alpha=0$, *i.e.* that in the absence of repulsive interactions, drops quite sharply to zero at very low overvoltage, which indicates that the repulsive interaction deduced quantum-mechanically[12], is essential to reveal the experimental aspects of τ. On the other hand, τ calculated by the proportional approximation follows the observed ones fairly well for $\alpha=4.4$ on the basis of (110)–lattice plane in conformity with $\log i_+\sim\eta$ relation referred to in (3), §5–3. The same explanation as that in (4), §5–3, applies to the curious behaviour of τ on (111)–lattice plane of assuming a negative value at higher overvoltages as shown in Fig. 13.

DISCUSSION

One of the present authors showed[7] as mentioned in the Introduction that the experimental results on the hydrogen electrode reaction on nickel is theoretically reproduced as based on the (110)–lattice plane by taking into account repulsive interactions among hydrogen atoms both adsorbed and constituting the critical complex by the proportional approximation, where the potentials

of exchange repulsion was multiplied by a factor α of 4.4, suggesting the existence of saturation current, *ca.* 2×10^{2} A cm^{-2} at 25°C and 1 atm H_2. The latter current has been recently confirmed experimentally by one of the present authors and YAMAZAKI[22] at the expected value in the concentrated solution of NaOH at 22±1°C. The adsorption isotherm of hydrogen on the (110)-lattice plane of Ni was deduced, on the other hand, theoretically by the second approximation mentioned in the Introduction, which was found in the best agreement at $\alpha=1.5$ with experimental results on Ni powder at 0.01~100 mmHg pressure of hydrogen. It is readily shown that the thermodynamic activity of hydrogen adatoms at the above mentioned pressures amounts to that in partial equilibrium of the step (3.a) at the overvoltage of $-0.288\sim-0.053$V.

The present analysis by the combined approximation shows that at such a low pressure, hydrogen adsorption takes place predominantly on (110)-lattice plane as shown in Fig. 8a, leaving the other lattice planes, especially (111)-lattice plane practically bare. In case where the hydrogen electrode is cathodically polarized to a certain extent, however, these lattice planes are no longer left bare. Thus at 0.4V of overvoltage corresponding to 10^{16} mmHg pressure of hydrogen, arround which the TAFEL law is almost closely obeyed as observed[22], the (110)-lattice plane is already completely covered, while the other lattice planes are covered to an appreciable extent as shown in Fig. 8a. It follows that the increase of current density is effected by that of the (100)- or (111)-lattice plane of higher energy of adatoms along with the increase of their activity, hence of the overvoltage, while the (110)-lattice plane of the lowest energy of adatom, which plays alternatively the leading part at lower activity of adatoms as in case of the adsorption isotherm mentioned above, is practically fully occupied to contribute just a constant, unimportant amount to the total current density. From a comparison of the theoretical calculation of $\log i_{+}\sim\eta$ or $\tau\sim\eta$ plot with the experimental results, it is concluded that the value of $\alpha=1.5$ gives the best coincidence between them as shown in Figs. 11 and 13 in accordance with the conclusion[11] independently arrived at.

The repulsive potentials depend now on the geometry of the lattice plane. An adatom on the (110)-lattice plane has only two nearest neighbours at $\theta=1$, while an adatom on the (100)- or (111)-lattice plane has four or six such neighbours respectively. Hence the repulsive potential on the (111)-lattice plane is roughly three times as large as that on the (110)-lattice plane. It is now understandable that the value of $\alpha=4.4$ adequately accounts for the observed TAFEL line as based on the (110)-lattice plane[7], whereas in the present case, the value $\alpha=1.5$ confirmed by the analysis of adsorption isotherms[11], fits in with experimental results with due regard to the (100)- and (111)-lattice planes involved.

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References

1) J. TAFEL, Z. physik. Chem., **50**, 641 (1905).
2) R. PARSONS, *Handbook of Electrochemical Constants*, Butterworths Scientific Publications, London, 1959.
3) K. J. VETTER, *Electrochemische Kinetik*, Springer-Verlag, Berlin, 1961.
4) I. LANGMUIR, Trans. Faraday Soc., **17**, 621 (1922).
5) G. OKAMOTO, J. HORIUTI and K. HIROTA, Sci. Papers Inst. Phys. Chem. Research (Tokyo), **29**, 223 (1936).
6) W. L. BRAGG and E. J. WILLIAMS, Proc. Roy. Soc. (London), **A 145**, 699 (1936).
7) J. HORIUTI, This Journal, **4**, 55 (1956-7).
8) T. KWAN, This Journal, **1**, 81 (1948-51); *Advances in Catalysis*, **6**, 67, Academic Press, New York, (1954).
9) J. HORIUTI and K. HIROTA, This Journal, **8**, 51 (1960).
10) H. A. BETHE, Proc. Roy. Soc. (London), **A 150**, 552 (1935).
R. E. PEIERLS, Proc. Cambridge Phil. Soc., **32**, 471 (1936).
11) J. HORIUTI and T. TOYA, This Journal, **12**, 76 (1964).
12) T. TOYA, *ibid.*,; **6**, 308 (1958); **8**, 211 (1960).
13) J. HORIUTI, *ibid.*, **11**, 55 (1963).
14) J. HORIUTI, *ibid.*, **1**, 8 (1948-51).
15) T. TOYA and J. HORIUTI, *Kinetics and Catalysis*, USSR, **4**, 3 (1963).
16) L. H. GERMER and A. U. MACREA, J. Chem. Phys., **37**, 1382 (1962).
L. H. GERMER, E. J. SCHEIBNER and C. D. HARTMANN, Phil Mag., **5**, 222 (1960).
L. H. GERMER and C. D. HARTMANN, J. Phys. Chem. Solid, **14**, 75 (1960).
17) R. WORTMAN, R. GOMER and R. LUNDY, J. Chem. Phys., **27**, 1099 (1957).
18) N. ROSEN and S. IKEHARA, Phys. Rev., **43**, 5 (1933).
19) *Cf.* S. GLASSTONE, K. J. LAIDLER and H. EYRING, *The Theory of Rate Processes*, p. 121, McGraw-Hill Book Co., New York, 1941.
20) J. O'M. BOCKRIS and S. SRINIVASAN, J. Electrochem. Soc., **111**, 858 (1964).
21) LANDOLT, *Tabellen* IIIc, p. 2349 (1936).
22) H. KITA and T. YAMAZAKI, This Journal, **11**, 10 (1963).

APPENDIX

The following tables show all of the possible arrangements of hydrogen adatoms of all possible numbers inside $\sum$ and the corresponding terms of the sums of Eqs. (IV. 15). The notation of solid circle or [≒] represents a hydrogen adatom or an critical complex and g the weight of a given arrangement respectively.

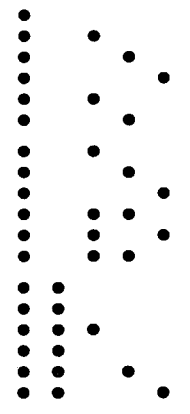
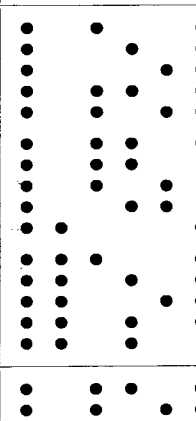
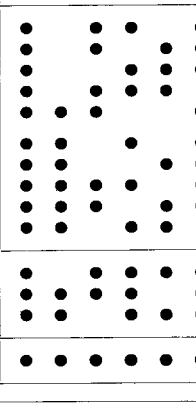
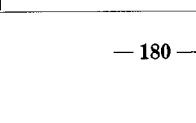
TABLE I. $\Omega C_{\sigma_1(\mathrm{H})}$, $\Omega C_{\sigma_1(0)}$ and $\Omega C_{\sigma_4(0)}$ on (110)-lattice plane

		Arrangement in $\sum$, *i.e.* 						Values of g, L, U, V, W, S and T in Eq. (IV. 16)							g
		σ_1	σ_2	σ_3	σ_4	σ_5	σ_6	g	L	U	V	W	S	T	
$\Omega C_{\sigma_1(\mathrm{H})}$	$\Omega C_{\sum\{\sigma_1(\mathrm{H}),5\sigma(0)\}}$	●						0	0	0	0	0	1	2	1
	$\Omega C_{\sum\{\sigma_1(\mathrm{H}),5\sigma(\mathrm{H})\}}$	●			●			1	1	1	0	0	2	5	2
		●		●				1	1	0	0	1	2	5	2
		●	●					1	0	0	1	0	2	4	1
	$\Omega C_{\sum\{\sigma_1(\mathrm{H}),5\sigma(2\mathrm{H})\}}$	●		●	●			2	2	1	1	1	3	8	2
		●			●	●		2	2	2	0	0	3	8	1
		●		●			●	2	2	0	0	2	3	8	1
		●	●	●				2	1	1	1	1	3	7	2
		●	●		●			2	1	1	1	1	3	7	2
		●			●		●	2	2	1	0	1	3	8	2
	$\Omega C_{\sum\{\sigma_1(\mathrm{H}),5\sigma(3\mathrm{H})\}}$	●	●	●	●			3	2	2	2	2	4	10	2
		●	●		●	●		3	2	2	1	2	4	10	2
		●	●	●		●		3	2	2	1	2	4	10	2
		●			●	●	●	3	3	2	1	1	4	11	2
		●		●		●	●	3	3	1	1	2	4	11	2
	$\Omega C_{\sum\{\sigma_1(\mathrm{H}),5\sigma(4\mathrm{H})\}}$	●	●	●	●		●	4	3	3	2	3	5	13	2
		●	●		●	●	●	4	3	3	2	3	5	13	2
		●		●	●	●	●	4	4	2	2	2	5	14	1
	$\Omega C_{\sum\{\sigma_1(\mathrm{H}),5\sigma(5\mathrm{H})\}}$	●	●	●	●	●	●	5	4	4	3	4	6	16	1
$\Omega C_{\sigma_1(0)}$	$\Omega C_{\sum\{\sigma_1(0),5\sigma(0)\}}$							0	0	0	0	0	0	0	1
	$\Omega C_{\sum\{\sigma_1(0),5\sigma(\mathrm{H})\}}$				●			1	1	0	0	0	1	3	4
			●					1	0	0	0	0	1	2	1
	$\Omega C_{\sum\{\sigma_1(0),5\sigma(2\mathrm{H})\}}$			●	●			2	2	0	1	0	2	6	2
					●	●		2	2	0	0	0	2	6	2
			●	●				2	1	1	0	0	2	5	2
			●		●			2	1	0	0	1	2	5	2
				●		●		2	2	0	0	0	2	6	2
	$\Omega C_{\sum\{\sigma_1(0),5\sigma(3\mathrm{H})\}}$		●	●	●			3	2	1	1	1	3	8	2
				●	●		●	3	3	0	1	0	3	9	2
			●		●	●		3	2	0	0	2	3	8	1
			●	●			●	3	2	2	0	0	3	8	1
			●		●		●	3	2	1	0	1	3	8	2
				●	●	●		3	3	0	1	0	3	9	2

$\mathfrak{A}C_{\sigma_1(0)}$	$\mathfrak{A}C_{\sum\{\sigma_1(0),5\sigma(4H)\}}$	●	●	●		●	4	3	2	1	1	4	11	2
			●	●	●	●	4	4	0	2	0	4	12	1
		●	●	●	●		4	3	1	1	2	4	11	2
	$\mathfrak{A}C_{\sum\{\sigma_1(0),5\sigma(5H)\}}$	●	●	●	●	●	5	4	2	2	2	5	14	1
$\mathfrak{A}C_{\sigma_4(0)}$	$\mathfrak{A}C_{\sum\{\sigma_4(0),5\sigma(0)\}}$						0	0	0	0	0	0	0	1
	$\mathfrak{A}C_{\sum\{\sigma_4(0),5\sigma(H)\}}$		●				1	1	0	0	0	1	3	3
				●			1	0	0	0	0	1	2	2
	$\mathfrak{A}C_{\sum\{\sigma_4(0),5\sigma(2H)\}}$		●	●			2	1	1	0	0	2	5	3
				●		●	2	2	0	0	0	2	6	1
				●	●		2	2	0	0	0	2	6	1
		●	●				2	0	0	1	0	2	4	1
					●	●	2	2	0	1	0	2	6	1
			●		●		2	1	0	0	1	2	5	3
	$\mathfrak{A}C_{\sum\{\sigma_4(0),5\sigma(3H)\}}$		●	●		●	3	2	2	0	0	3	8	1
				●	●	●	3	3	0	1	0	3	9	1
		●		●		●	3	2	0	0	2	3	8	1
		●			●	●	3	2	1	1	1	3	8	2
		●	●			●	3	1	1	1	1	3	7	3
			●	●		●	3	2	1	0	1	3	8	2
	$\mathfrak{A}C_{\sum\{\sigma_4(0),5\sigma(4H)\}}$		●	●		●	4	3	2	1	1	4	11	1
		●	●			●	4	2	2	2	2	4	10	1
		●	●	●		●	4	2	2	1	2	4	10	1
		●	●	●			4	2	2	1	2	4	10	1
		●		●		●	4	3	1	1	2	4	11	1
	$\mathfrak{A}C_{\sum\{\sigma_4(0),5\sigma(5H)\}}$	●	●	●		●	5	3	3	2	3	5	13	1

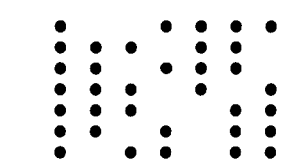
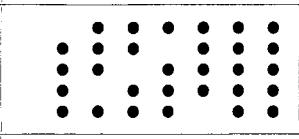
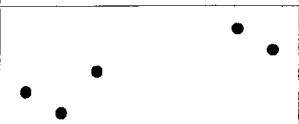
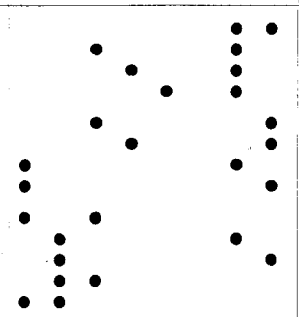
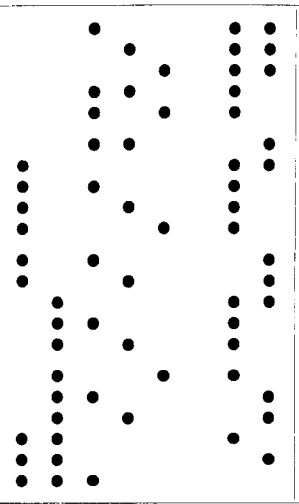
TABLE II. $\mathfrak{A}C_{\sigma_1(H)}$, $\mathfrak{A}C_{\sigma_1(0)}$, $\mathfrak{A}C_{\sigma_6(0)}$ and $\mathfrak{A}C_{\sigma_7(0)}$ on (100)-lattic plane

		Arrangement in $\sum$, *i. e.* 								Values of g, M, N, U, V and S in Eq. (IV. 20)						$\mathfrak{g}$
		σ_1	σ_2	σ_3	σ_4	σ_5	σ_6	σ_7	σ_8	g	M	N	U	V	S	
$\mathfrak{A}C_{\sigma_1(H)}$	$\mathfrak{A}C_{\sum\{\sigma_1(H),7\sigma(0)\}}$	●								0	0	0	0	0	2	1
	$\mathfrak{A}C_{\sum\{\sigma_1(H),7\sigma(H)\}}$	●					●			1	0	1	1	0	4	1
		●						●		1	1	0	1	0	4	2
		●							●	1	1	0	0	1	4	2
		●		●						1	0	1	0	0	4	1
		●	●							1	0	0	1	0	4	1
	$\mathfrak{A}C_{\sum\{\sigma_1(H),7\sigma(2H)\}}$	●					●	●		2	1	1	2	1	6	2
		●					●		●	2	1	1	1	1	6	2
		●		●			●			2	0	2	1	0	6	1
		●						●	●	2	2	0	2	1	6	2
		●		●				●		2	1	1	1	0	6	2
		●			●			●		2	2	0	1	1	6	2
		●				●		●		2	2	0	2	0	6	1
		●		●					●	2	1	1	0	2	6	2
		●			●				●	2	2	0	0	2	6	1
		●	●				●			2	0	1	2	0	6	2
		●	●					●		2	1	0	2	1	6	4

$\Sigma C_{\sigma_1(H)}$	$\Sigma C_{\Sigma\{\sigma_1(H),7\sigma(3H)\}}$		3	2	1	3	2	8	2
			3	1	2	2	1	8	2
			3	2	1	2	2	8	2
			3	2	1	3	2	8	1
			3	1	2	1	2	8	2
			3	2	1	1	2	8	1
			3	2	1	2	2	8	2
			3	3	0	2	2	8	2
			3	3	0	3	1	8	2
			3	2	1	1	2	8	2
			3	2	1	2	0	8	1
			3	2	1	0	4	8	1
			3	1	1	3	2	8	4
			3	1	1	3	1	8	4
			3	0	2	3	0	8	1
			3	2	0	4	2	8	2
			3	2	0	3	2	8	2
			3	2	0	3	2	8	2
	$\Sigma C_{\Sigma\{\sigma_1(H),7\sigma(4H)\}}$		4	2	2	3	3	10	2
			4	3	1	3	3	10	2
			4	3	1	4	3	10	2
			4	2	2	2	3	10	2
			4	2	2	3	2	10	1
			4	2	2	1	4	10	1
			4	3	1	2	4	10	2
			4	3	1	3	2	10	2
			4	4	0	4	2	10	1
			4	2	1	5	3	10	4
			4	1	2	4	2	10	4
			4	2	1	4	3	10	4
			4	2	1	4	4	10	2
			4	2	1	4	2	10	2
			4	3	0	5	3	10	4
	$\Sigma C_{\Sigma\{\sigma_1(H),7\sigma(5H)\}}$		5	3	2	3	5	12	2
			5	3	2	4	4	12	2
			5	4	1	5	4	12	1
			5	4	1	4	4	12	1
			5	2	2	6	4	12	2
			5	3	1	6	4	12	4
			5	3	1	6	5	12	4
			5	2	2	5	4	12	2
			5	2	2	5	4	12	2
			5	4	0	7	4	12	1
	$\Sigma C_{\Sigma\{\sigma_1(H),7\sigma(6H)\}}$		6	4	2	5	6	14	1
			6	3	2	7	6	14	4
			6	4	1	8	6	14	2
	$\Sigma C_{\Sigma\{\sigma_1(H),7\sigma(7H)\}}$		7	4	2	9	8	16	1
$\Sigma C_{\sigma_1(0)}$	$\Sigma C_{\Sigma\{\sigma_1(0),7\sigma(0)\}}$		0	0	0	0	0	0	1
	$\Sigma C_{\Sigma\{\sigma_1(0),7\sigma(H)\}}$		1	0	1	0	0	2	1
			1	1	0	0	0	2	2
			1	1	0	0	0	2	2
			1	0	1	0	0	2	1
			1	0	0	0	0	2	1

$\mathfrak{Q}C_{\sigma_1(0)}$

$\mathfrak{Q}C_{\Sigma\{\sigma_1(0),7\sigma(2H)\}}$	2	1	1	0	1	4	2
	2	1	1	0	0	4	2
	2	0	2	0	0	4	1
	2	2	0	1	0	4	2
	2	1	1	0	0	4	2
	2	2	0	0	0	4	2
	2	2	0	0	0	4	1
	2	1	1	0	1	4	2
	2	2	0	0	0	4	1
	2	0	1	0	0	4	1
	2	1	0	0	1	4	2
	2	1	0	1	0	4	2
	2	0	1	1	0	4	1
$\mathfrak{Q}C_{\Sigma\{\sigma_1(0),7\sigma(3H)\}}$	3	2	1	1	1	6	2
	3	1	2	0	1	6	2
	3	2	1	0	1	6	2
	3	2	1	0	2	6	1
	3	1	2	0	1	6	2
	3	2	1	0	0	6	1
	3	2	1	1	1	6	2
	3	3	0	1	0	6	2
	3	3	0	1	0	6	2
	3	2	1	0	1	6	2
	3	2	1	0	0	6	1
	3	2	1	0	2	6	1
	3	1	1	0	2	6	2
	3	1	1	1	0	6	2
	3	0	2	1	0	6	1
	3	2	0	2	1	6	2
	3	1	1	1	1	6	2
	3	2	0	1	1	6	2
	3	2	0	0	2	6	1
	3	1	1	2	1	6	2
	3	2	0	2	0	6	1
$\mathfrak{Q}C_{\Sigma\{\sigma_1(0),7\sigma(4H)\}}$	4	2	2	1	2	8	2
	4	3	1	1	1	8	2
	4	3	1	1	2	8	2
	4	2	2	0	2	8	2
	4	2	2	0	2	8	1
	4	2	2	0	2	8	1
	4	3	1	1	2	8	2
	4	3	1	1	1	8	2
	4	4	0	2	0	8	1
	4	2	1	2	2	8	2
	4	1	2	1	2	8	2
	4	2	1	1	2	8	2
	4	2	1	0	4	8	1
	4	1	2	2	1	8	2
	4	2	1	2	0	8	1
	4	2	1	3	2	8	2
	4	3	0	3	1	8	2
	4	3	0	2	2	8	2
	4	2	1	2	2	8	2
	4	2	1	1	2	8	1
	4	2	1	3	2	8	1
$\mathfrak{Q}C_{\Sigma\{\sigma_1(0),7\sigma(5H)\}}$	5	3	2	1	3	10	4
	5	4	1	2	2	10	2
	5	2	2	3	3	10	2
	5	3	1	3	2	10	2

$\mathfrak{A}C_{\sigma_1(0)}$	$\mathfrak{A}C_{\Sigma\{\sigma_1(0),7\sigma(5H)\}}$		5	3	1	2	4	10	2
			5	2	2	2	3	10	2
			5	2	2	1	4	10	1
			5	2	2	3	2	10	1
			5	3	1	4	3	10	2
			5	3	1	3	3	10	2
			5	4	0	4	2	10	1
	$\mathfrak{A}C_{\Sigma\{\sigma_1(0),7\sigma(6H)\}}$		6	4	2	2	4	12	1
			6	3	2	4	4	12	2
			6	3	2	3	5	12	2
			6	4	1	4	4	12	1
			6	4	1	5	4	12	1
	$\mathfrak{A}C_{\Sigma\{\sigma_1(0),7\sigma(7H)\}}$		7	4	2	5	6	14	1
$\mathfrak{A}C_{\sigma_6(0)}$	$\mathfrak{A}C_{\Sigma\{\sigma_6(0),7\sigma(0)\}}$		0	0	0	0	0	0	1
	$\mathfrak{A}C_{\Sigma\{\sigma_6(0),7\sigma(H)\}}$		1	1	0	0	0	2	2
			1	1	0	0	0	2	2
			1	0	1	0	0	2	1
			1	0	0	0	0	2	1
			1	0	0	0	0	2	1
	$\mathfrak{A}C_{\Sigma\{\sigma_6(0),7\sigma(2H)\}}$		2	2	0	1	0	4	2
			2	1	1	0	0	4	2
			2	2	0	0	0	4	2
			2	2	0	0	0	4	1
			2	1	1	0	1	4	2
			2	2	0	0	0	4	1
			2	1	0	1	0	4	2
			2	1	0	0	1	4	2
			2	0	1	0	0	4	1
			2	1	0	0	1	4	2
			2	1	0	1	0	4	2
			2	0	1	1	0	4	1
			2	0	0	1	0	4	1
	$\mathfrak{A}C_{\Sigma\{\sigma_6(0),7\sigma(3H)\}}$		3	2	1	1	1	6	2
			3	3	0	1	0	6	2
			3	3	0	1	0	6	2
			3	2	1	0	1	6	2
			3	2	1	0	0	6	1
			3	2	1	0	2	6	1
			3	2	0	2	1	6	2
			3	1	1	1	0	6	2
			3	2	0	1	1	6	2
			3	2	0	2	0	6	1
			3	1	1	0	2	6	2
			3	2	0	0	2	6	1
			3	2	0	2	1	6	2
			3	1	1	1	1	6	2
			3	2	0	1	1	6	2
			3	2	0	0	2	6	1
			3	1	1	2	1	6	2
			3	2	0	2	0	6	1
			3	1	0	2	1	6	2
			3	1	0	2	1	6	2
			3	0	1	2	0	6	1

$\mathfrak{A}C_{\sigma_6(0)}$	$\mathfrak{A}C_{\Sigma\{\sigma_6(0),7\sigma(4H)\}}$	●	●	●	●			●	●	4	3	1	1	2	8	2
		●	●			●		●	●	4	3	1	1	1	8	2
		●		●		●		●	●	4	4	0	2	0	8	1
			●	●				●	●	4	2	1	2	2	8	2
			●		●			●	●	4	3	0	2	2	8	2
				●		●		●	●	4	3	0	3	1	8	2
				●	●			●		4	2	1	1	2	8	2
				●		●		●		4	2	1	2	0	8	1
				●	●				●	4	2	1	0	4	8	1
			●	●				●	●	4	2	1	3	2	8	2
			●		●			●	●	4	3	0	3	1	8	2
			●			●		●	●	4	3	0	2	2	8	2
			●	●	●			●		4	2	1	2	2	8	2
			●	●		●		●		4	2	1	1	2	8	1
			●	●	●				●	4	2	1	3	2	8	1
		●	●					●	●	4	2	0	4	2	8	2
		●	●	●				●		4	1	1	3	1	8	2
		●	●		●			●		4	2	0	3	2	8	2
		●	●			●		●		4	2	0	3	2	8	1
		●	●	●					●	4	1	1	3	2	8	2
		●	●		●				●	4	2	0	3	2	8	1
	$\mathfrak{A}C_{\Sigma\{\sigma_6(0),7\sigma(5H)\}}$	●		●	●	●		●	●	5	4	1	2	2	10	1
		●		●	●			●	●	5	3	1	2	4	10	2
		●		●		●		●	●	5	3	1	3	2	10	2
		●			●	●		●	●	5	4	0	4	2	10	1
			●	●	●			●	●	5	3	1	4	3	10	2
			●	●		●		●	●	5	3	1	3	3	10	2
			●		●	●		●	●	5	4	0	4	2	10	1
		●	●	●				●	●	5	2	1	5	3	10	2
		●	●		●			●	●	5	3	0	5	3	10	2
		●	●			●		●	●	5	3	0	5	3	10	2
		●	●	●	●			●		5	2	1	4	3	10	2
		●	●	●		●		●		5	2	1	4	2	10	1
		●	●	●	●				●	5	2	1	4	4	10	1
	$\mathfrak{A}C_{\Sigma\{\sigma_6(0),7\sigma(6H)\}}$	●		●	●	●		●	●	6	4	1	4	4	12	1
		●	●	●	●			●	●	6	3	1	6	5	12	2
		●	●	●		●		●	●	6	3	1	6	4	12	2
		●	●		●	●		●	●	6	4	0	7	4	12	1
			●	●	●	●		●	●	6	4	1	5	4	12	1
	$\mathfrak{A}C_{\Sigma\{\sigma_6(0),7\sigma(7H)\}}$	●	●	●	●	●		●	●	7	4	1	8	6	14	1
$\mathfrak{A}C_{\sigma_7(0)}$	$\mathfrak{A}C_{\Sigma\{\sigma_7(0),7\sigma(0)\}}$									0	0	0	0	0	0	1
	$\mathfrak{A}C_{\Sigma\{\sigma_7(0),7\sigma(H)\}}$						●			1	0	1	0	0	2	2
									●	1	1	0	0	0	2	2
						●				1	1	0	0	0	2	1
		●								1	0	0	0	0	2	2
	$\mathfrak{A}C_{\Sigma\{\sigma_7(0),7\sigma(2H)\}}$						●		●	2	1	1	0	0	4	2
				●			●			2	0	2	0	0	4	1
						●	●			2	1	1	0	1	4	1
				●					●	2	1	1	0	1	4	2
					●				●	2	2	0	0	0	4	1
						●			●	2	2	0	0	0	4	1
				●		●				2	1	1	0	0	4	1
					●	●				2	2	0	1	0	4	1
		●					●			2	0	1	1	0	4	2
		●							●	2	1	0	0	1	4	2

$\mathfrak{A}C_{\sigma_7(0)}$	$\mathfrak{A}C_{\Sigma\{\sigma_7(0),7\sigma(2H)\}}$	2	0	1	0	0	4	2
		2	1	0	1	0	4	2
		2	1	0	1	0	4	1
		2	1	0	0	1	4	1
		2	0	0	1	0	4	1
	$\mathfrak{A}C_{\Sigma\{\sigma_7(0),7\sigma(3H)\}}$	3	1	2	0	1	6	3
		3	2	1	0	0	6	1
		3	2	1	0	1	6	2
		3	2	1	0	2	6	1
		3	3	0	1	0	6	1
		3	2	1	1	1	6	2
		3	1	1	1	1	6	3
		3	0	2	1	0	6	2
		3	1	1	2	1	6	3
		3	1	1	0	2	6	3
		3	2	0	0	2	6	1
		3	2	0	1	1	6	2
		3	1	1	1	0	6	3
		3	2	0	2	1	6	2
		3	2	0	2	0	6	1
		3	0	1	2	0	6	2
		3	1	0	2	1	6	3
	$\mathfrak{A}C_{\Sigma\{\sigma_7(0),7\sigma(4H)\}}$	4	2	2	0	2	8	1
		4	2	2	0	2	8	1
		4	3	1	1	1	8	1
		4	2	2	1	2	8	1
		4	3	1	1	2	8	1
		4	1	2	1	2	8	3
		4	2	1	1	2	8	1
		4	2	1	2	2	8	2
		4	1	2	2	1	8	3
		4	2	1	3	2	8	2
		4	2	1	0	4	8	1
		4	2	1	1	2	8	2
		4	3	0	2	2	8	1
		4	2	1	2	2	8	2
		4	2	1	2	0	8	1
		4	2	1	3	2	8	1
		4	3	0	3	1	8	1
		4	1	1	3	1	8	3
		4	0	2	3	0	8	1
		4	1	1	3	2	8	3
		4	2	0	3	2	8	1
		4	2	0	3	2	8	1
		4	2	0	4	2	8	1
	$\mathfrak{A}C_{\Sigma\{\sigma_7(0),7\sigma(5H)\}}$	5	3	2	1	3	10	1
		5	2	2	1	4	10	1
		5	2	2	2	3	10	2
		5	3	1	3	3	10	1
		5	2	2	3	3	10	2
		5	3	1	2	4	10	1
		5	2	2	3	2	10	1
		5	3	1	3	2	10	1
		5	3	1	4	3	10	1
		5	1	2	4	2	10	3
		5	2	1	4	2	10	1
		5	2	1	4	3	10	2
		5	2	1	5	3	10	2
		5	2	1	4	4	10	1
		5	3	0	5	3	10	1

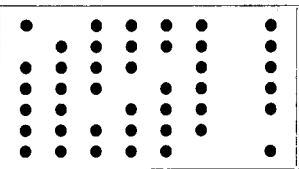
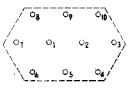
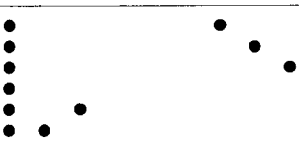
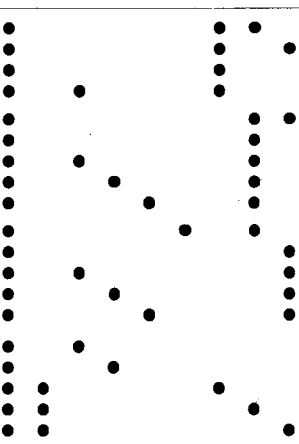
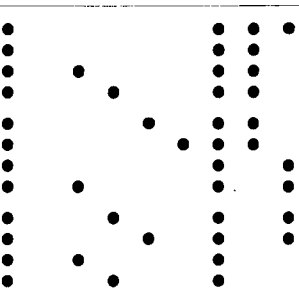
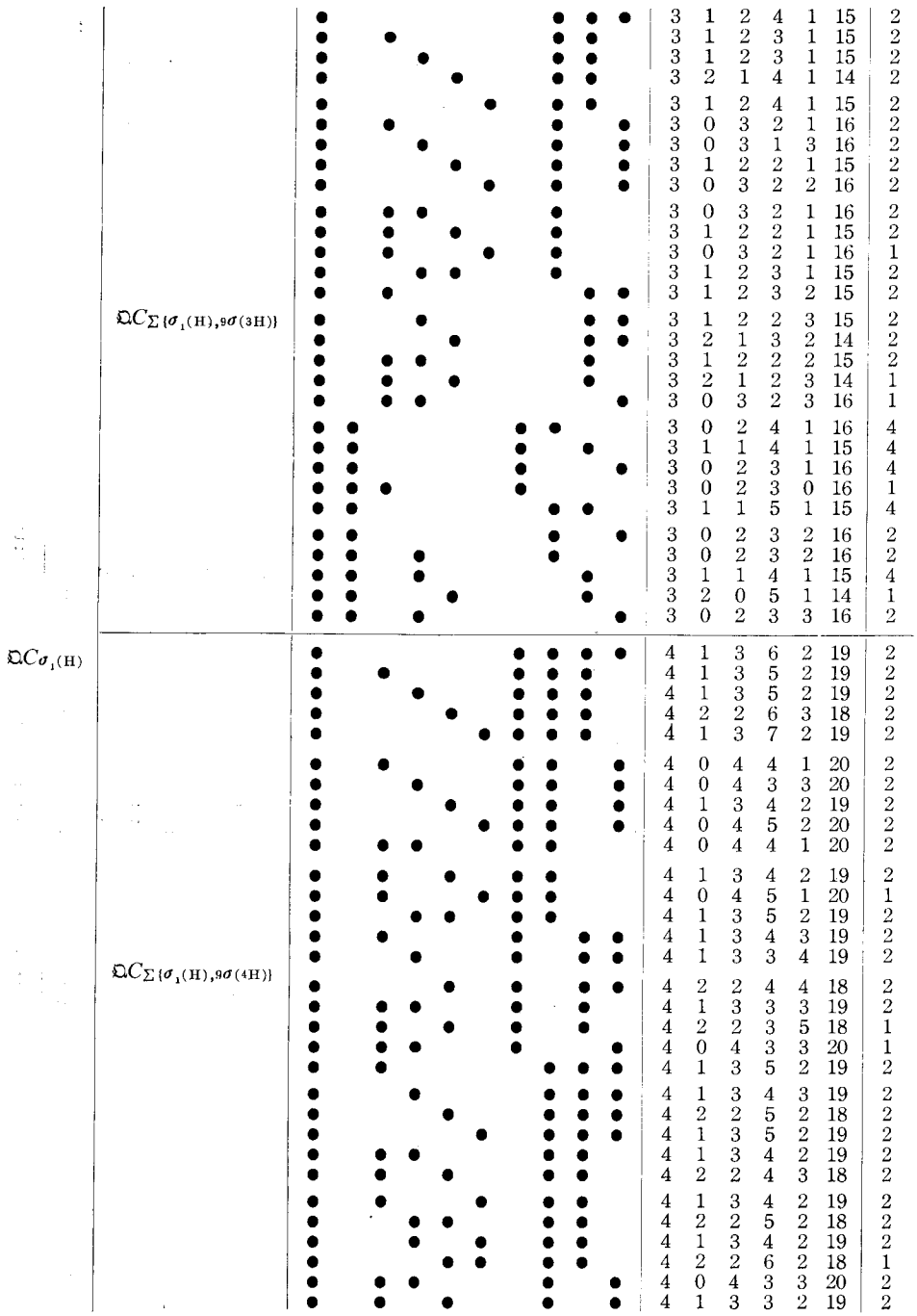
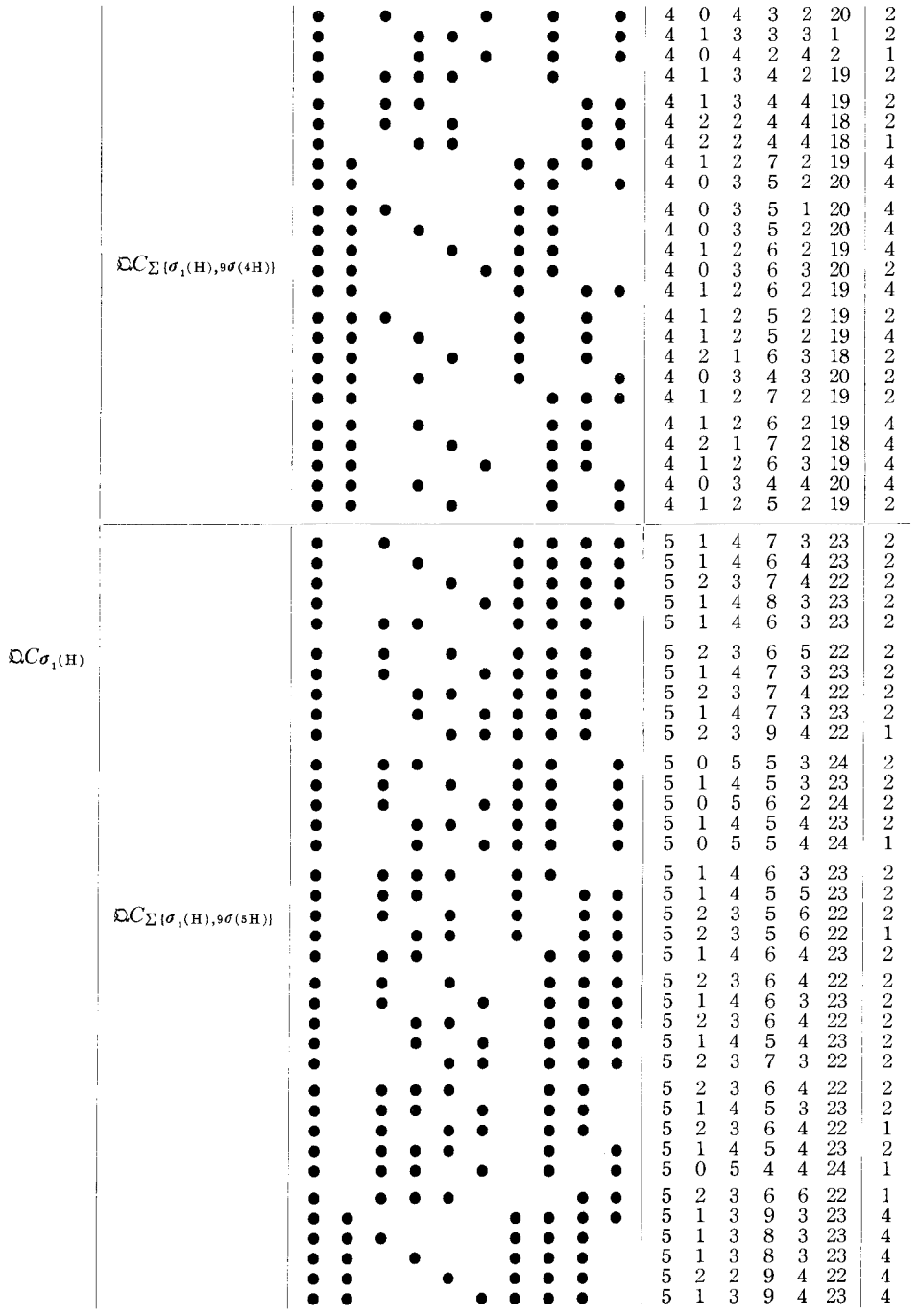
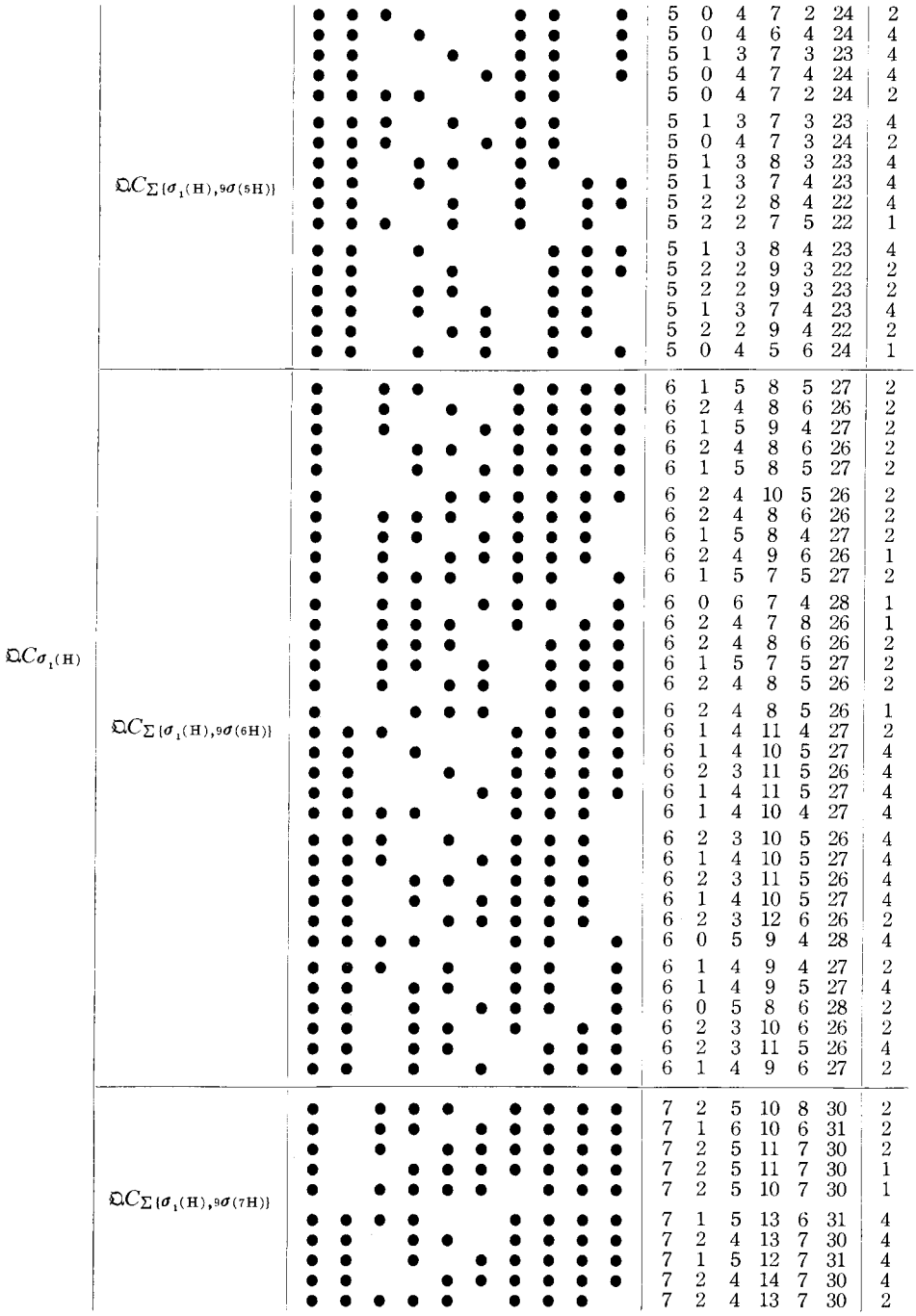
$\mathfrak{Q}C_{\sigma_7(0)}$	$\mathfrak{Q}C_{\sum\{\sigma_7(0),7\sigma(6H)\}}$		6	3	2	3	5	12	1
			6	3	2	4	4	12	1
			6	2	2	5	4	12	1
			6	2	2	5	4	12	1
			6	3	1	6	4	12	1
			6	2	2	6	4	12	1
			6	3	1	6	5	12	1
	$\mathfrak{Q}C_{\sum\{\sigma_7(0),7\sigma(7H)\}}$		7	3	2	7	6	14	1

TABLE III. $\mathfrak{Q}C_{\sigma_1(H)}$, $\mathfrak{Q}C_{\sigma_1(0)}$, $\mathfrak{Q}C_{\sigma_8(0)}$ and $\mathfrak{Q}C_{\sigma_9(0)}$ on (111)-lattice plane

		Arrangement in $\sum$, *i. e.* 	Values of g, M, N, U, W and T in Eq. (IV. 25)						g
		σ_1 σ_2 σ_3 σ_4 σ_5 σ_6 σ_7 σ_8 σ_9 σ_{10}	g	M	N	U	W	T	
$\mathfrak{Q}C_{\sigma_1(H)}$	$\mathfrak{Q}C_{\sum\{\sigma_1(H),9\sigma(0)\}}$		0	0	0	0	0	4	1
	$\mathfrak{Q}C_{\sum\{\sigma_1(H),9\sigma(H)\}}$		1	0	1	1	0	8	1
			1	0	1	1	0	8	2
			1	1	0	1	0	7	2
			1	0	1	0	1	8	2
			1	0	1	0	0	8	1
			1	0	0	1	0	8	1
	$\mathfrak{Q}C_{\sum\{\sigma_1(H),9\sigma(2H)\}}$		2	0	2	3	0	12	2
			2	1	1	2	1	11	2
			2	0	2	1	1	12	2
			2	0	2	1	0	12	1
			2	1	1	3	0	11	2
			2	0	2	1	1	12	2
			2	0	2	1	0	12	2
			2	0	2	1	1	12	2
			2	1	1	2	0	11	2
			2	0	2	2	1	12	1
			2	1	1	2	1	11	2
			2	1	1	1	1	11	2
			2	1	1	1	1	11	2
			2	2	0	2	1	10	1
			2	0	2	1	1	12	2
			2	0	2	0	3	12	1
			2	0	1	2	0	12	2
			2	0	1	2	1	12	4
			2	1	0	3	0	11	2
	$\mathfrak{Q}C_{\sum\{\sigma_1(H),9\sigma(3H)\}}$		3	1	2	5	1	15	2
			3	0	3	3	1	16	2
			3	0	3	3	0	16	2
			3	0	3	3	1	16	2
			3	1	2	4	1	15	2
			3	0	3	5	1	16	1
			3	1	2	3	2	15	2
			3	1	2	2	2	15	2
			3	1	2	2	2	15	2
			3	2	1	3	3	14	1
			3	0	3	2	1	16	2
			3	0	3	1	3	16	1


$\mathfrak{A}C_{\Sigma\{\sigma_1(H),9\sigma(3H)\}}$
$\mathfrak{A}C_{\sigma_1(H)}$
$\mathfrak{A}C_{\Sigma\{\sigma_1(H),9\sigma(4H)\}}$

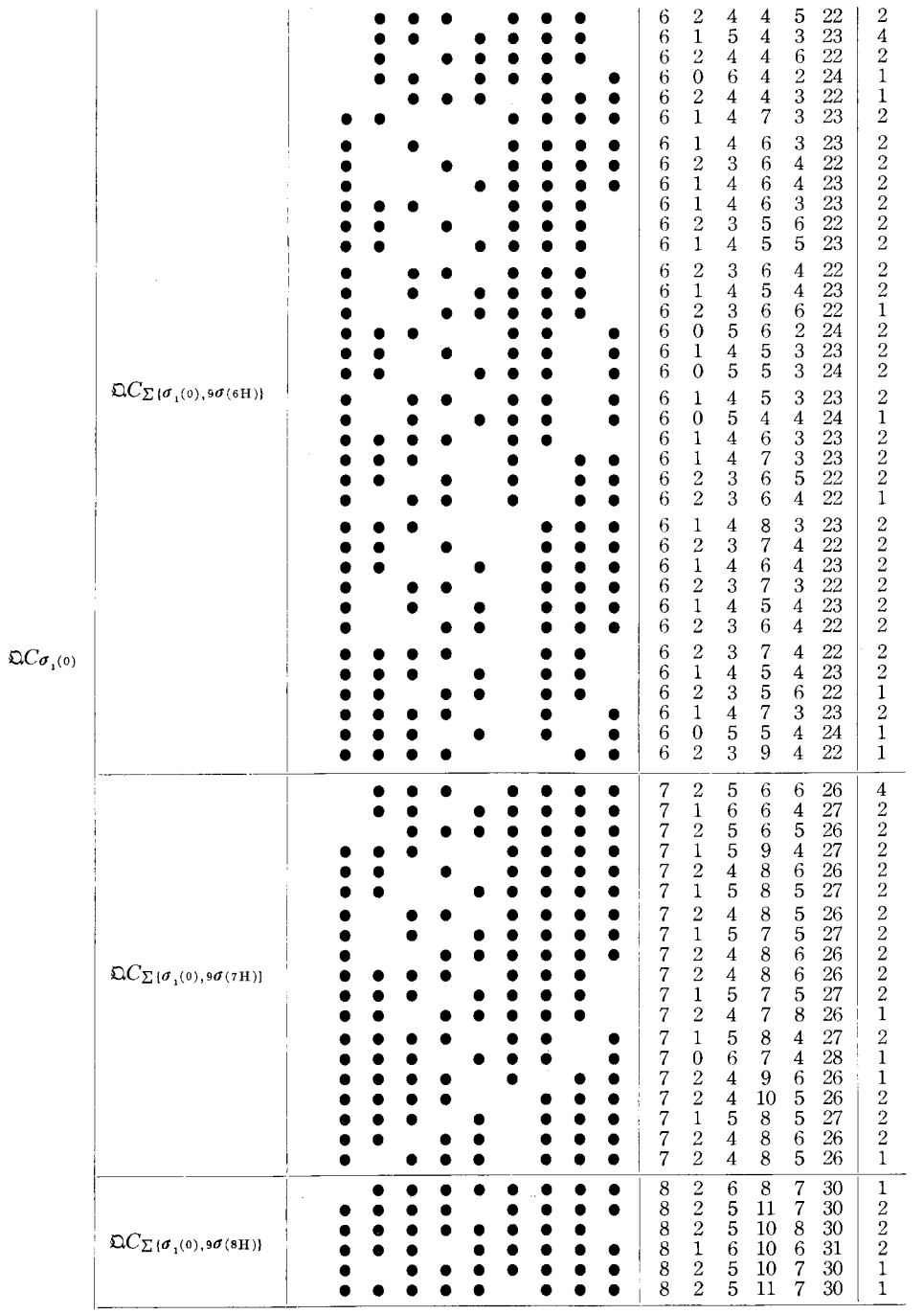

$\Sigma C_{\Sigma\{\sigma_1(H),9\sigma(4H)\}}$
$\Sigma C_{\sigma_1(H)}$
$\Sigma C_{\Sigma\{\sigma_1(H),9\sigma(5H)\}}$


$\mathfrak{Q}C_{\sigma_1(H)}$
$\mathfrak{Q}C_{\Sigma\{\sigma_1(H),9\sigma(5H)\}}$
$\mathfrak{Q}C_{\Sigma\{\sigma_1(H),9\sigma(6H)\}}$
$\mathfrak{Q}C_{\Sigma\{\sigma_1(H),9\sigma(7H)\}}$

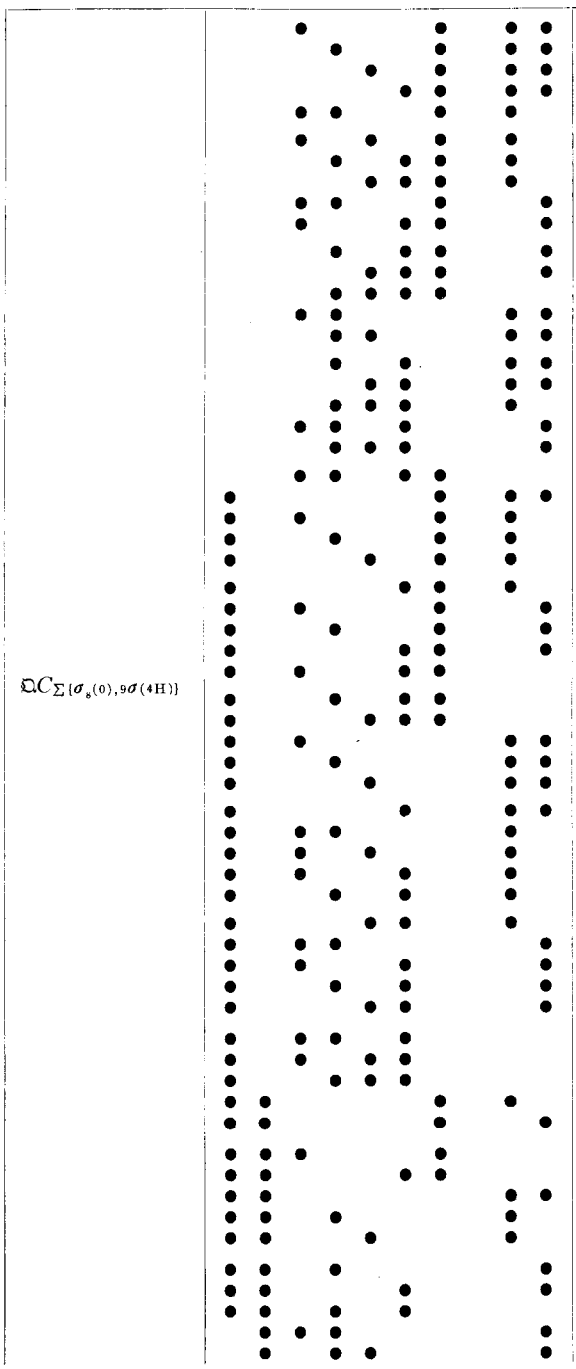
$\mathfrak{A}C_{\sigma_1(\mathrm{H})}$	$\mathfrak{A}C_{\sum\{\sigma_1(\mathrm{H}),9\sigma(7\mathrm{H})\}}$	●	●	●	●		●	●	●	●		7	1	5	12	6	31	4
		●	●	●		●	●	●	●	●		7	2	4	13	8	30	2
		●	●	●	●		●	●	●		●	7	0	6	11	6	32	1
		●	●		●	●	●		●	●	●	7	2	4	13	7	30	1
		●	●	●		●		●	●	●	●	7	2	4	13	7	30	2
	$\mathfrak{A}C_{\sum\{\sigma_1(\mathrm{H}),9\sigma(8\mathrm{H})\}}$	●		●	●	●	●	●	●	●	●	8	2	6	13	9	34	1
		●	●	●	●	●		●	●	●	●	8	2	5	16	9	34	4
		●	●	●	●		●	●	●	●	●	8	1	6	15	8	35	2
		●	●		●	●	●	●	●	●	●	8	2	5	16	9	34	2
	$\mathfrak{A}C_{\sum\{\sigma_1(\mathrm{H}),9\sigma(9\mathrm{H})\}}$	●	●	●	●	●	●	●	●	●	●	9	2	6	19	11	38	1
$\mathfrak{A}C_{\sigma_1(0)}$	$\mathfrak{A}C_{\sum\{\sigma_1(0),9\sigma(0)\}}$											0	0	0	0	0	0	1
	$\mathfrak{A}C_{\sum\{\sigma_1(0),9\sigma(\mathrm{H})\}}$							●				1	0	1	0	0	4	6
										●		1	1	0	0	0	3	2
			●									1	0	0	0	0	4	1
	$\mathfrak{A}C_{\sum\{\sigma_1(0),9\sigma(2\mathrm{H})\}}$							●	●			2	0	2	1	0	8	4
								●		●		2	1	1	0	1	7	4
								●			●	2	0	2	0	0	8	4
				●				●				2	0	2	0	0	8	1
								●	●			2	1	1	1	0	7	4
								●			●	2	0	2	0	0	8	2
				●				●				2	0	2	0	0	8	2
					●			●				2	1	1	0	0	7	4
						●		●				2	0	2	0	1	8	2
					●					●		2	2	0	0	1	6	1
		●						●				2	0	1	0	0	8	1
		●						●				2	0	1	0	1	8	2
		●								●		2	1	0	1	0	7	2
		●									●	2	0	1	1	0	8	3
	$\mathfrak{A}C_{\sum\{\sigma_1(0),9\sigma(3\mathrm{H})\}}$							●	●			3	1	2	2	1	11	4
								●	●		●	3	0	3	1	0	12	4
				●				●	●			3	0	3	1	0	12	4
					●			●	●			3	0	3	1	0	12	4
								●	●			3	1	2	1	1	11	4
						●		●	●			3	0	3	2	1	12	2
								●		●	●	3	1	2	1	1	11	4
				●				●		●		3	1	2	0	2	11	2
					●			●		●		3	1	2	0	1	11	4
								●		●		3	2	1	0	3	10	2
					●			●			●	3	0	3	0	1	12	2
									●	●	●	3	1	2	2	0	11	2
				●					●	●		3	1	2	1	0	11	4
					●				●	●		3	2	1	1	1	10	4
						●			●	●		3	1	2	1	1	11	4
				●					●		●	3	0	3	0	1	12	4
					●				●		●	3	1	2	0	0	11	2
		●						●	●			3	0	2	1	1	12	2
		●						●		●		3	1	1	1	1	11	2
		●						●			●	3	0	2	1	0	12	2
		●						●				3	0	2	1	0	12	1
		●							●	●		3	1	1	2	1	11	2
		●							●		●	3	0	2	1	1	12	2
		●		●					●			3	0	2	1	1	12	2
		●			●				●			3	0	2	1	1	12	2
		●				●			●			3	1	1	1	1	11	2
		●							●			3	0	2	0	3	12	1
		●								●	●	3	1	1	3	0	11	2

	$\mathfrak{Q}C_{\Sigma\{\sigma_1(0),9\sigma(3H)\}}$	●	●						●		3	1	1	2	1	11	2
		●		●					●		3	1	1	2	0	11	2
		●			●				●		3	2	0	2	1	10	1
		●	●							●	3	0	2	3	0	12	2
		●		●						●	3	0	2	2	1	12	1
$\mathfrak{Q}C_{\sigma_1(0)}$	$\mathfrak{Q}C_{\Sigma\{\sigma_1(0),9\sigma(4H)\}}$						●	●	●	●	4	1	3	3	1	15	4
			●				●	●	●		4	1	3	2	2	15	4
				●			●	●	●		4	1	3	2	1	15	4
					●		●	●	●		4	2	2	2	3	14	4
						●	●	●	●		4	1	3	3	2	15	4
			●				●	●		●	4	0	4	2	0	16	2
				●			●	●		●	4	0	4	1	1	16	4
					●		●	●		●	4	1	3	1	1	15	4
						●	●	●		●	4	0	4	2	1	16	4
			●	●			●	●			4	0	4	2	0	16	2
			●		●		●	●			4	1	3	1	2	15	4
			●			●	●	●			4	0	4	2	1	16	2
				●	●		●	●			4	1	3	2	1	15	4
				●			●		●	●	4	1	3	1	2	15	4
					●		●		●	●	4	2	2	1	3	14	4
			●		●		●		●		4	2	2	0	5	14	1
				●				●	●	●	4	1	3	2	1	15	4
					●			●	●	●	4	2	2	2	1	14	2
				●	●			●	●		4	2	2	2	1	14	2
				●		●		●	●		4	1	3	1	1	15	4
					●	●		●	●		4	2	2	2	2	14	2
				●		●		●		●	4	0	4	0	2	16	1
		●					●	●	●		4	1	2	3	2	15	2
		●					●	●		●	4	0	3	2	1	16	2
		●	●				●	●			4	0	3	2	1	16	2
		●		●			●	●			4	0	3	2	1	16	2
		●			●		●	●			4	1	2	2	2	15	2
		●				●	●	●			4	0	3	2	3	16	1
		●					●		●	●	4	1	2	3	1	15	2
		●	●				●		●		4	1	2	2	2	15	2
		●		●			●		●		4	1	2	2	1	15	2
		●			●		●		●		4	2	1	2	3	14	1
		●	●				●			●	4	0	3	3	0	16	2
		●		●			●			●	4	0	3	2	1	16	1
		●						●	●	●	4	1	2	4	1	15	2
		●	●					●	●		4	1	2	3	2	15	2
		●		●				●	●		4	1	2	3	1	15	2
		●			●			●	●		4	2	1	3	2	14	2
		●				●		●	●		4	1	2	2	3	15	2
		●	●					●		●	4	0	3	3	1	16	2
		●		●				●		●	4	0	3	2	2	16	2
		●			●			●		●	4	1	2	2	1	15	2
		●				●		●		●	4	0	3	1	3	16	2
		●	●	●				●			4	0	3	3	1	16	2
		●	●		●			●			4	1	2	2	2	15	2
		●	●			●		●			4	0	3	1	3	16	1
		●		●	●			●			4	1	2	3	1	15	2
		●	●						●	●	4	1	2	5	1	15	2
		●		●					●	●	4	1	2	4	1	15	2
		●			●				●	●	4	2	1	4	1	14	2
		●	●	●					●		4	1	2	4	1	15	2
		●	●		●				●		4	2	1	3	3	14	1
		●	●	●						●	4	0	3	5	1	16	1

$\mathfrak{Q}C_{\sigma_1(0)}$	$\mathfrak{Q}C_{\Sigma\{\sigma_1(0),9\sigma(5H)\}}$		●				●	●	●	●	5	1	4	4	2	19	2
				●			●	●	●	●	5	1	4	3	2	19	4
					●		●	●	●	●	5	2	3	3	3	18	4
						●	●	●	●	●	5	1	4	4	2	19	4
			●	●			●	●	●		5	1	4	3	2	19	4
			●		●		●	●	●		5	2	3	2	5	18	4
			●			●	●	●	●		5	1	4	3	3	19	4
				●	●		●	●	●		5	2	3	3	3	18	4
				●		●	●	●	●		5	1	4	3	2	19	4
					●	●	●	●	●		5	2	3	4	4	18	2
			●	●			●	●		●	5	0	5	3	1	20	4
			●		●		●	●		●	5	1	4	2	2	19	2
				●	●		●	●		●	5	1	4	2	2	19	4
				●		●	●	●		●	5	0	5	2	2	20	2
				●	●		●		●	●	5	2	3	2	4	18	2
				●	●			●	●	●	5	2	3	3	2	18	4
				●		●		●	●	●	5	1	4	2	2	19	2
		●					●	●	●	●	5	1	3	5	2	19	2
		●	●				●	●	●		5	1	3	4	3	19	2
		●		●			●	●	●		5	1	3	4	2	19	2
		●			●		●	●			5	2	2	4	4	18	2
		●				●	●	●	●		5	1	3	4	4	19	2
		●	●				●	●		●	5	0	4	4	1	20	2
		●		●			●	●		●	5	0	4	3	2	20	2
		●			●		●	●		●	5	1	3	3	2	19	2
		●				●	●	●		●	5	0	4	3	3	20	2
		●	●	●			●	●			5	0	4	4	1	20	2
		●	●		●		●	●			5	1	3	3	3	19	2
		●	●			●	●	●			5	0	4	3	3	20	1
		●		●	●		●	●			5	1	3	4	2	19	2
		●	●				●		●	●	5	1	3	5	2	19	2
		●		●			●		●	●	5	1	3	4	2	19	2
		●			●		●		●	●	5	2	2	4	3	18	2
		●	●	●			●		●		5	1	3	4	2	19	2
		●	●		●		●		●		5	2	2	3	5	18	1
		●	●	●			●			●	5	0	4	5	1	20	1
		●	●					●	●	●	5	1	3	6	2	19	2
		●		●				●	●	●	5	1	3	5	2	19	2
		●			●			●	●	●	5	2	2	5	2	18	2
		●				●		●	●	●	5	1	3	4	3	19	2
		●	●	●				●	●		5	1	3	5	2	19	2
		●	●		●			●	●		5	2	2	4	4	18	2
		●	●			●		●	●		5	1	3	3	4	19	2
		●		●	●			●	●		5	2	2	5	2	18	2
		●		●		●		●	●		5	1	3	3	3	19	2
		●			●	●		●	●		5	2	2	4	4	18	1
		●	●	●				●		●	5	0	4	5	2	20	2
		●	●		●			●		●	5	1	3	4	2	19	2
		●	●			●		●		●	5	0	4	3	3	20	2
		●		●	●			●		●	5	1	3	4	2	19	2
		●			●	●		●		●	5	0	4	2	4	20	1
		●	●	●	●			●			5	1	3	5	2	19	2
		●	●	●					●	●	5	1	3	7	2	19	2
		●	●		●				●	●	5	2	2	6	3	18	2
		●		●	●				●	●	5	2	2	6	2	18	1
	$\mathfrak{Q}C_{\Sigma\{\sigma_1(0),9\sigma(6H)\}}$		●	●			●	●	●	●	6	1	5	5	3	23	4
			●		●		●	●	●	●	6	2	4	4	5	22	2
				●	●		●	●	●	●	6	2	4	4	4	22	4
				●		●	●	●	●	●	6	1	5	4	3	23	4
					●	●	●	●	●	●	6	2	4	5	4	22	4

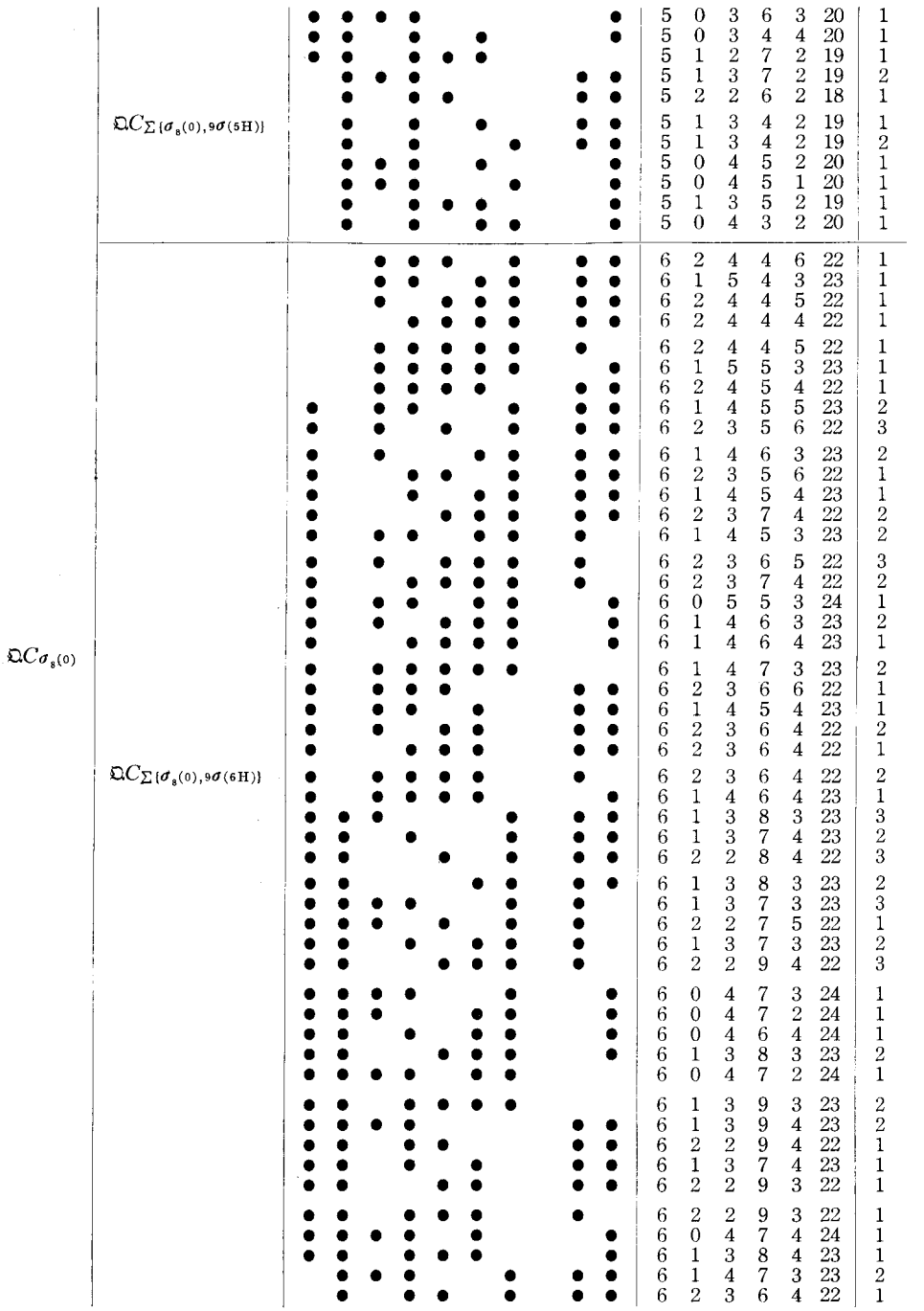

ΩC_Σ{σ_1(0),9σ(6H)}
ΩC_σ1(0)
ΩC_Σ{σ_1(0),9σ(7H)}
ΩC_Σ{σ_1(0),9σ(8H)}

	$\Sigma C_{\Sigma\{\sigma_1(0),9\sigma(9H)\}}$	●	●	●	●	●	●	●	●	●	9	2	6	13	9	34	1
$\Sigma C_{\sigma_8(0)}$	$\Sigma C_{\Sigma\{\sigma_8(0),9\sigma(0)\}}$										0	0	0	0	0	0	1
	$\Sigma C_{\Sigma\{\sigma_8(0),9\sigma(H)\}}$						●		●		1	0	1	0	0	4	5
											1	1	0	0	0	3	2
		●									1	0	0	0	0	4	2
	$\Sigma C_{\Sigma\{\sigma_8(0),9\sigma(2H)\}}$						●		●		2	1	1	0	1	7	4
							●			●	2	0	2	0	0	8	3
				●			●				2	0	2	0	0	8	1
						●	●				2	0	2	1	0	8	3
									●	●	2	1	1	1	0	7	3
				●					●		2	1	1	0	0	7	3
					●				●		2	2	0	0	1	6	1
				●						●	2	0	2	0	1	8	1
						●				●	2	0	2	0	0	8	1
				●		●					2	0	2	0	0	8	1
		●					●				2	0	1	1	0	8	5
		●							●		2	1	0	1	0	7	4
		●								●	2	0	1	0	1	8	3
		●		●							2	0	1	0	0	8	2
		●	●								2	0	0	1	0	8	1
	$\Sigma C_{\Sigma\{\sigma_8(0),9\sigma(3H)\}}$						●		●	●	3	1	2	1	1	11	3
				●			●		●		3	1	2	0	2	11	2
					●		●		●		3	1	2	0	1	11	3
						●	●		●		3	2	1	0	3	10	2
					●		●		●		3	1	2	1	1	11	3
				●			●			●	3	0	3	1	0	12	3
					●		●			●	3	0	3	0	1	12	1
						●	●			●	3	0	3	1	0	12	2
				●			●				3	0	3	1	0	12	2
					●	●	●				3	1	2	2	1	11	3
				●					●	●	3	1	2	1	1	11	2
					●				●	●	3	2	1	1	1	10	3
						●			●	●	3	1	2	1	0	11	2
				●		●			●		3	1	2	0	0	11	1
			●	●						●	3	0	3	2	1	12	1
				●		●				●	3	0	3	0	1	12	1
				●	●	●					3	1	2	2	0	11	1
		●					●		●		3	1	1	2	1	11	4
		●					●			●	3	0	2	1	1	12	3
		●		●			●				3	0	2	1	0	12	2
		●				●	●				3	0	2	3	0	12	3
		●							●	●	3	1	1	2	1	11	3
		●		●					●		3	1	1	1	1	11	4
		●			●				●		3	1	1	1	1	11	3
		●				●			●		3	2	0	2	1	10	2
		●					●		●		3	1	1	2	0	11	3
		●		●						●	3	0	2	1	1	12	3
		●			●					●	3	0	2	0	3	12	1
		●				●				●	3	0	2	1	1	12	2
		●		●		●					3	0	2	1	0	12	3
		●			●	●					3	0	2	1	1	12	2
		●			●	●					3	1	1	3	0	11	3
		●	●				●				3	0	1	2	0	12	2
		●	●						●		3	1	0	3	0	11	2
		●	●							●	3	0	1	2	1	12	3
			●		●					●	3	0	2	2	1	12	1



$\mathfrak{Q}C_{\sigma_s(0)}$	$\mathfrak{Q}C_{\Sigma\{\sigma_s(0),9\sigma(4H)\}}$														
		4	1	3	2	2	15	3
		4	1	3	1	2	15	2
		4	2	2	1	3	14	3
		4	1	3	2	1	15	2
		4	1	3	1	2	15	3
		4	2	2	0	5	14	1
		4	1	3	1	1	15	2
		4	2	2	2	3	14	3
		4	0	4	2	1	16	1
		4	0	4	2	0	16	1
		4	0	4	1	1	16	1
		4	1	3	2	1	15	2
		4	1	3	3	1	15	2
		4	1	3	3	2	15	2
		4	2	2	2	2	14	1
		4	1	3	1	1	15	1
		4	2	2	2	1	14	1
		4	2	2	2	1	14	1
		4	0	4	2	1	16	1
		4	1	3	2	1	15	1
		4	0	4	2	0	16	1
		4	1	2	3	2	15	3
		4	1	2	2	2	15	4
		4	1	2	2	2	15	3
		4	2	1	3	3	14	2
		4	1	2	4	1	15	3
		4	0	3	2	1	16	3
		4	0	3	1	3	16	1
		4	0	3	3	1	16	2
		4	0	3	3	0	16	3
		4	0	3	3	1	16	2
		4	1	2	5	1	15	3
		4	1	2	3	2	15	3
		4	1	2	2	3	15	2
		4	2	1	3	2	14	3
		4	1	2	3	1	15	2
		4	1	2	2	2	15	3
		4	2	1	2	3	14	2
		4	1	2	2	1	15	3
		4	1	2	2	1	15	2
		4	2	1	4	1	14	3
		4	0	3	2	3	16	1
		4	0	3	2	1	16	2
		4	0	3	1	3	16	1
		4	1	2	3	1	15	2
		4	0	3	2	1	16	2
		4	1	2	3	1	15	3
		4	1	2	4	1	15	2
		4	1	1	4	1	15	4
		4	0	2	3	1	16	3
		4	0	2	3	0	16	1
		4	0	2	4	1	16	3
		4	1	1	5	1	15	3
		4	1	1	4	1	15	3
		4	2	0	5	1	14	1
		4	0	2	3	3	16	1
		4	0	2	3	2	16	1
		4	0	2	3	2	16	1
		4	0	3	5	1	16	1
		4	1	2	4	1	15	2

			●		●		●				●	4	0	3	2	2	16	1
			●		●			●			●	4	0	3	2	1	16	1
$\mathfrak{Q}C_{\sigma_8(0)}$	$\mathfrak{Q}C_{\Sigma\{\sigma_8(0),9\sigma(5H)\}}$			●	●			●		●	●	5	1	4	3	3	19	2
				●		●		●		●	●	5	2	3	2	5	18	3
				●			●	●		●	●	5	1	4	3	2	19	2
					●	●		●		●	●	5	2	3	2	4	18	1
					●		●	●		●	●	5	1	4	2	2	19	1
						●	●	●		●	●	5	2	3	3	3	18	2
				●	●		●	●		●		5	1	4	2	2	19	1
					●	●	●	●		●		5	2	3	3	3	18	2
				●	●		●	●			●	5	0	5	3	1	20	1
					●	●	●	●			●	5	1	4	3	2	19	1
				●	●	●	●	●				5	1	4	4	2	19	1
				●	●	●				●	●	5	2	3	4	4	18	1
				●	●		●			●	●	5	1	4	3	2	19	1
					●	●	●			●	●	5	2	3	3	2	18	1
				●	●	●	●				●	5	1	4	4	2	19	1
		●		●				●		●	●	5	1	3	4	3	19	3
		●			●			●		●	●	5	1	3	3	4	19	2
		●				●		●		●	●	5	2	2	4	4	18	3
		●					●	●		●	●	5	1	3	5	2	19	2
		●		●	●			●		●		5	1	3	3	3	19	3
		●		●		●		●		●		5	2	2	3	5	18	2
		●		●			●	●		●		5	1	3	4	2	19	3
		●			●		●	●		●		5	1	3	4	2	19	2
		●				●	●	●		●		5	2	2	6	3	18	3
		●		●	●			●			●	5	0	4	3	3	20	1
		●		●			●	●			●	5	0	4	4	1	20	2
		●			●		●	●			●	5	0	4	3	3	20	1
		●				●	●	●			●	5	1	3	5	2	19	2
		●		●	●		●	●				5	0	4	4	1	20	2
		●		●		●	●	●				5	1	3	5	2	19	3
		●			●	●	●	●				5	1	3	6	2	19	2
		●		●	●					●	●	5	1	3	4	4	19	2
		●		●		●				●	●	5	2	2	4	4	18	3
		●		●			●			●	●	5	1	3	4	2	19	2
		●			●	●				●	●	5	2	2	4	4	18	1
		●			●		●			●	●	5	1	3	3	3	19	1
		●				●	●			●	●	5	2	2	5	2	18	2
		●		●	●		●			●		5	1	3	3	2	19	2
		●		●		●	●			●		5	2	2	4	3	18	3
		●			●	●	●			●		5	2	2	5	2	18	2
		●		●	●		●				●	5	0	4	3	3	20	1
		●		●		●	●				●	5	1	3	4	2	19	2
		●			●	●	●				●	5	1	3	4	3	19	1
		●		●	●	●	●					5	1	3	5	2	19	2
		●	●					●		●	●	5	1	2	6	2	19	3
		●	●	●				●		●		5	1	2	5	2	19	2
		●	●		●			●		●		5	1	2	5	2	19	3
		●	●			●		●		●		5	2	1	6	3	18	2
		●	●				●	●		●		5	1	2	6	2	19	3
		●	●	●				●			●	5	0	3	5	1	20	3
		●	●		●			●			●	5	0	3	4	3	20	1
		●	●				●	●			●	5	0	3	5	2	20	2
		●	●		●		●	●				5	0	3	5	2	20	2
		●	●			●	●	●				5	1	2	7	2	19	3
		●	●		●					●	●	5	1	2	6	3	19	2
		●	●			●				●	●	5	2	1	7	2	18	3
		●	●				●			●	●	5	1	2	6	2	19	2
		●	●		●		●			●		5	1	2	5	2	19	1



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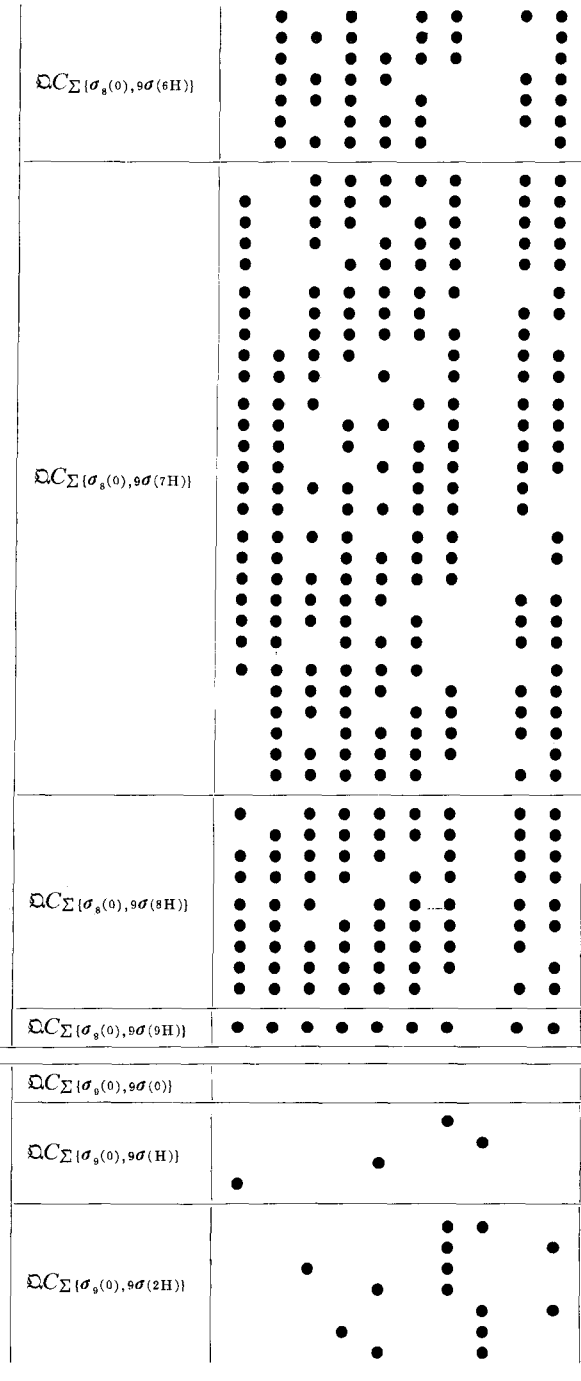
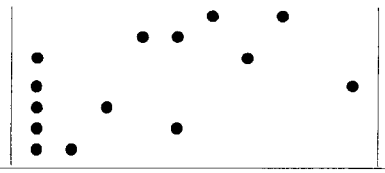
6	2	2	9	3	22	1
6	2	2	9	3	22	1
6	0	4	7	4	24	1
6	1	3	8	4	23	1
6	1	4	7	3	23	2
6	2	3	6	4	22	1



$\Sigma C_{\sigma_8(8)}$	$\Sigma C_{\Sigma\{\sigma_8(0),9\sigma(6H)\}}$	6	1	4	5	3	23	1
		6	0	5	6	2	24	1
		6	1	4	6	3	23	1
		6	2	3	9	4	22	1
		6	1	4	7	3	23	1
		6	2	3	7	3	24	1
		6	1	4	8	3	23	1
	$\Sigma C_{\Sigma\{\sigma_8(0),9\sigma(7H)\}}$	7	2	5	6	6	26	1
		7	2	4	7	8	26	1
		7	1	5	7	5	27	1
		7	2	4	8	6	26	2
		7	2	4	8	6	26	1
		7	1	5	8	5	27	1
		7	2	4	8	6	26	1
		7	2	4	8	6	26	2
		7	1	4	10	5	27	2
		7	2	3	10	6	26	3
		7	1	4	10	4	27	2
		7	2	3	10	6	26	1
		7	1	4	9	5	27	1
		7	2	3	11	5	26	2
		7	1	4	9	4	27	1
		7	2	3	11	5	26	2
		7	0	5	9	4	28	1
		7	1	4	10	5	27	1
		7	1	4	11	4	27	1
		7	2	3	12	6	26	1
		7	1	4	10	5	27	1
		7	2	3	11	5	26	1
		7	1	4	11	5	27	1
		7	2	4	9	6	26	1
		7	1	5	8	4	27	1
		7	2	4	8	5	26	1
		7	1	5	9	4	27	1
		7	2	4	10	5	26	1
	$\Sigma C_{\Sigma\{\sigma_8(0),9\sigma(8H)\}}$	8	2	5	10	8	30	1
		8	2	5	11	7	30	1
		8	2	4	13	8	30	1
		8	1	5	12	6	31	1
		8	2	4	13	7	30	1
		8	2	4	13	7	30	1
		8	2	4	13	7	30	1
		8	1	5	13	6	31	1
		8	2	4	14	7	30	1
	$\Sigma C_{\Sigma\{\sigma_8(0),9\sigma(9H)\}}$	9	2	5	16	9	34	1
$\Sigma C_{\sigma_9(0)}$	$\Sigma C_{\Sigma\{\sigma_9(0),9\sigma(0)\}}$	0	0	0	0	0	0	1
	$\Sigma C_{\Sigma\{\sigma_9(0),9\sigma(H)\}}$	1	0	1	0	0	4	2
		1	0	1	0	0	4	4
		1	1	0	0	0	3	1
		1	0	0	0	0	4	2
	$\Sigma C_{\Sigma\{\sigma_9(0),9\sigma(2H)\}}$	2	0	2	1	0	8	4
		2	0	2	0	0	8	4
		2	0	2	0	0	8	1
		2	1	1	0	1	7	2
		2	0	2	0	0	8	2
		2	0	2	0	0	8	2
		2	1	1	0	0	7	2

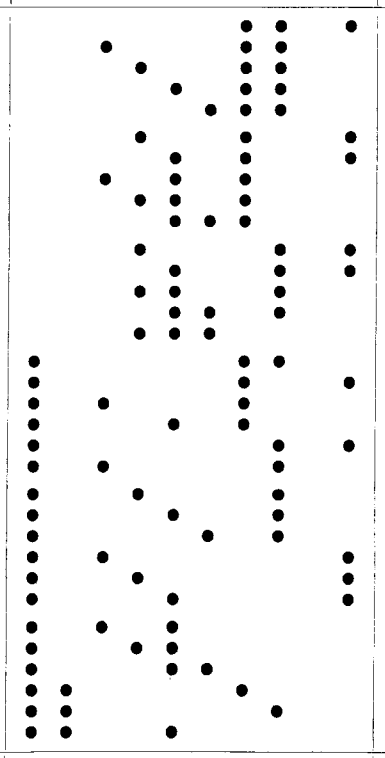
$\mathfrak{Q}C_{\sigma_9(0)}$

$\mathfrak{Q}C_{\Sigma\{\sigma_9(0),9\sigma(2H)\}}$



2	0	2	0	1	8	2
2	1	1	1	0	7	2
2	0	1	1	0	8	6
2	0	1	0	1	8	4
2	0	1	0	0	8	2
2	1	0	1	0	7	2
2	0	0	1	0	8	1

$\mathfrak{Q}C_{\Sigma\{\sigma_9(0),9\sigma(3H)\}}$



3	0	3	1	0	12	4
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3	1	2	1	1	11	2
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3	1	2	0	1	11	2
3	1	2	0	2	11	1
3	1	2	1	1	11	2
3	1	2	2	1	11	2
3	0	3	0	1	12	4
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3	1	2	1	0	11	2
3	1	2	1	1	11	2
3	1	2	2	0	11	1
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3	0	2	1	0	12	2
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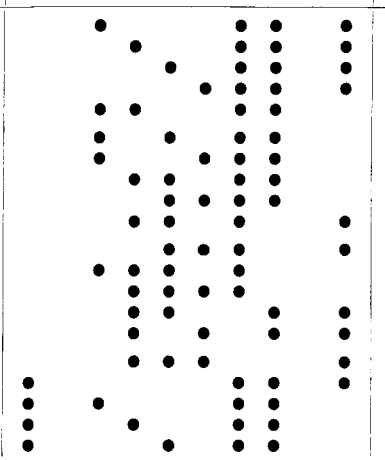
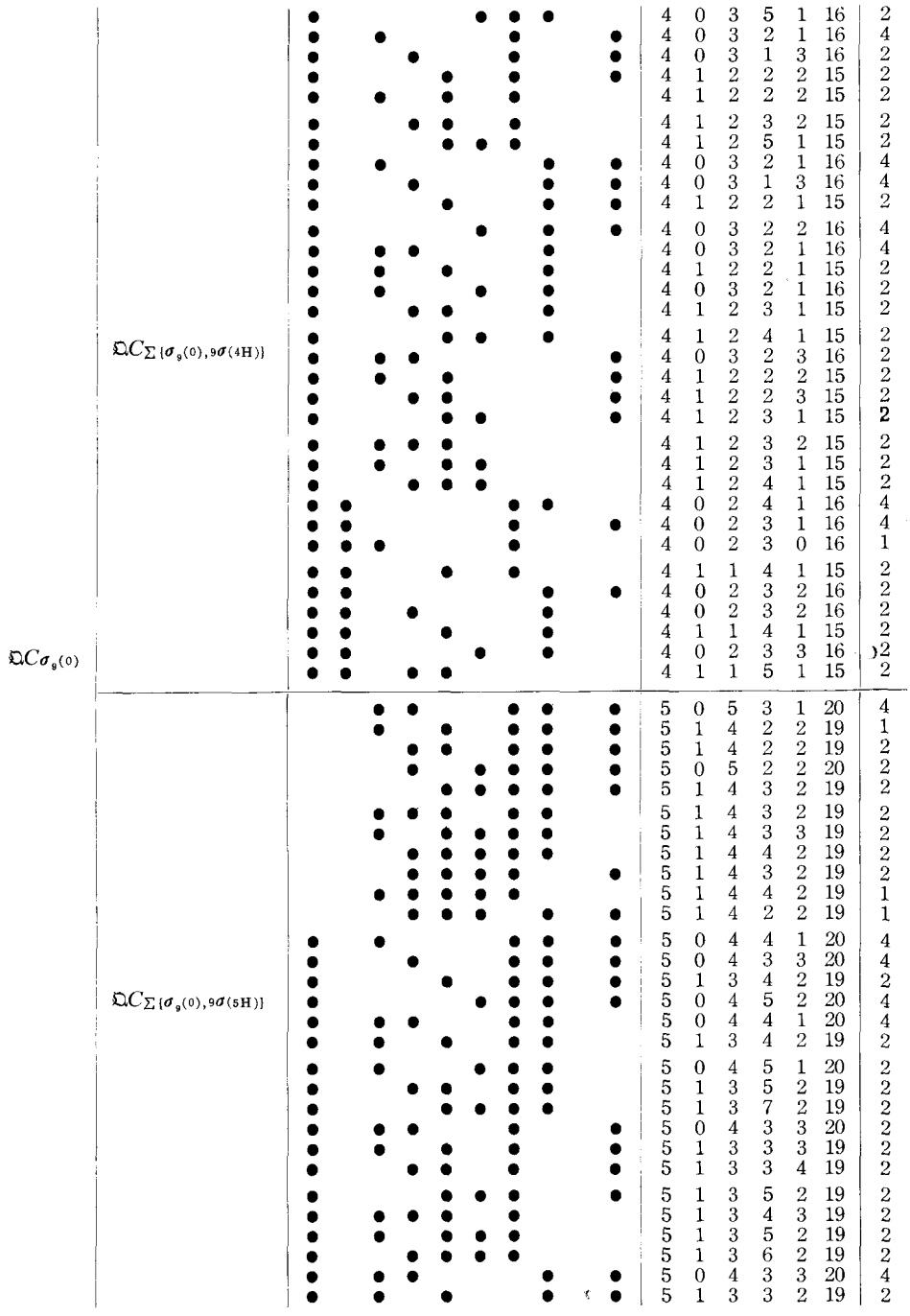
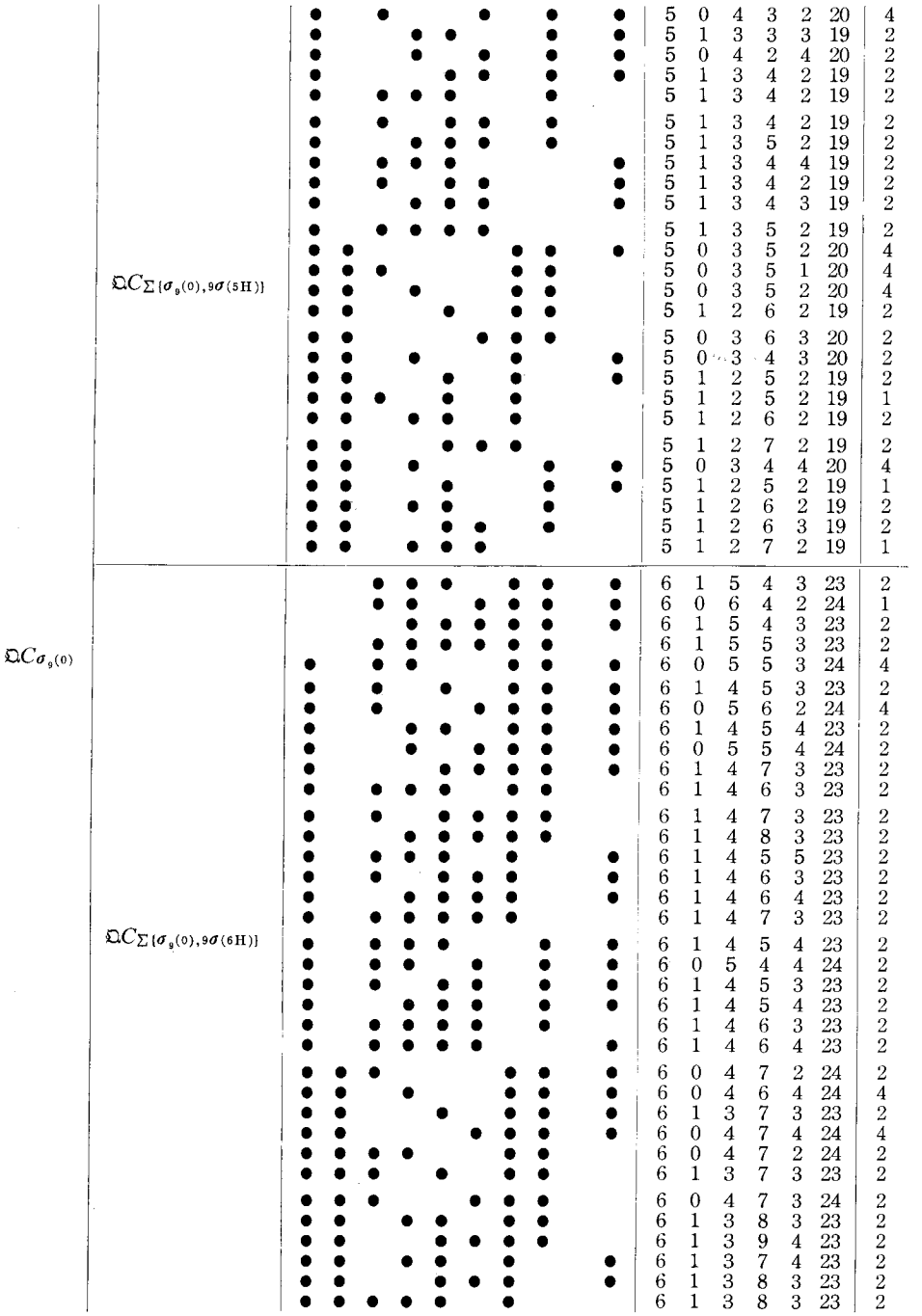
3	0	2	1	1	12	4
3	0	2	1	0	12	4
3	0	2	1	1	12	4
3	1	1	2	0	11	2
3	0	2	2	1	12	2
3	0	2	1	1	12	4
3	0	2	0	3	12	2
3	1	1	1	1	11	2
3	1	1	1	1	11	2
3	1	1	2	1	11	2
3	1	1	3	0	11	2
3	0	1	2	0	12	2
3	0	1	2	1	12	4
3	1	0	3	0	11	1

$\mathfrak{Q}C_{\Sigma\{\sigma_9(0),9\sigma(4H)\}}$



4	0	4	2	0	16	2
4	0	4	1	1	16	4
4	1	3	1	1	15	2
4	0	4	2	1	16	4
4	0	4	2	0	16	2
4	1	3	1	2	15	2
4	0	4	2	1	16	2
4	1	3	2	1	15	2
4	1	3	3	2	15	2
4	1	3	1	2	15	2
4	1	3	2	1	15	2
4	1	3	2	2	15	2
4	1	3	3	1	15	2
4	1	3	1	1	15	2
4	0	4	0	2	16	1
4	1	3	2	1	15	2
4	0	3	3	1	16	4
4	0	3	3	0	16	4
4	0	3	3	1	16	4
4	1	2	4	1	15	2

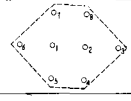

$\mathfrak{Q}C_{\Sigma\{\sigma_g(0),9\sigma(4H)\}}$
$\mathfrak{Q}C_{\sigma_g(0)}$
$\mathfrak{Q}C_{\Sigma\{\sigma_g(0),9\sigma(5H)\}}$


ΩC_Σ{σ_g(0),9σ(5H)}
ΩC_σg(0)
ΩC_Σ{σ_g(0),9σ(6H)}

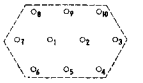
$\mathfrak{D}C_{\sigma_g(0)}$	$\mathfrak{D}C_{\Sigma\{\sigma_g(0),9\sigma(6H)\}}$	●	●		●	●		●		●	6	1	3	7	4	23	2
		●	●		●		●	●		●	6	0	4	5	6	24	1
		●	●		●	●	●			●	6	1	3	8	4	23	2
		●	●	●	●	●	●				6	1	3	9	3	23	2
	$\mathfrak{D}C_{\Sigma\{\sigma_g(0),9\sigma(7H)\}}$			●	●	●	●	●	●	●	7	1	6	6	4	27	1
		●		●	●	●		●	●	●	7	1	5	7	5	27	2
		●		●	●		●	●	●	●	7	0	6	7	4	28	2
		●		●		●	●	●	●	●	7	1	5	8	4	27	2
		●			●	●	●	●	●	●	7	1	5	8	5	27	2
		●		●	●	●	●	●	●		7	1	5	9	4	27	2
		●		●	●	●	●	●		●	7	1	5	8	5	27	2
		●		●	●	●	●		●	●	7	1	5	7	5	27	2
		●	●	●	●			●	●	●	7	0	5	9	4	28	4
		●	●	●		●		●	●	●	7	1	4	9	4	27	1
		●	●		●	●		●	●	●	7	1	4	9	5	27	2
		●	●		●		●	●	●	●	7	0	5	8	6	28	2
		●	●			●	●	●	●	●	7	1	4	10	5	27	2
		●	●	●	●	●		●	●		7	1	4	10	4	27	2
		●	●	●		●	●	●	●		7	1	4	10	5	27	2
		●	●		●	●	●	●	●		7	1	4	11	5	27	2
		●	●		●	●	●	●		●	7	1	4	10	5	27	2
		●	●	●	●	●	●	●			7	1	4	11	4	27	1
		●	●		●	●	●		●	●	7	1	4	9	6	27	1
	$\mathfrak{D}C_{\Sigma\{\sigma_g(0),9\sigma(8H)\}}$	●		●	●	●	●	●	●	●	8	1	6	10	6	31	2
		●	●	●	●	●		●	●	●	8	1	5	12	6	31	2
		●	●	●	●		●	●	●	●	8	0	6	11	6	32	1
		●	●		●	●	●	●	●	●	8	1	5	12	7	31	2
		●	●	●	●	●	●	●			8	1	5	13	6	31	2
	$\mathfrak{D}C_{\Sigma\{\sigma_g(0),9\sigma(9H)\}}$	●	●	●	●	●	●	●	●	●	9	1	6	15	8	35	1

TABLE IV. $\mathfrak{D}C^{\pm}_{\sigma^{\pm}(\pm)}$'s on (110)–, (100)– and (111)–lattice planes

		Arrangement in Σ, *i.e.* 						Values of g, L, V, S, T and U' in Eq. (V.3)						g
		σ_1	σ_2	σ_3	σ_4	σ_5	σ_6	g	L	V	S	T	U'	
$\mathfrak{D}C^{\pm}_{\sigma^{\pm}(\pm)}$	$[\pm]$							0	0	0	0	0	0	1
	$[\pm]$	●						1	1	0	1	3	1	4
	$[\pm]$	●				●		2	2	0	2	6	2	4
	$[\pm]$	●		●				2	2	1	2	6	2	2
	$[\pm]$	●		●		●		3	3	1	3	9	3	4
	$[\pm]$	●		●		●	●	4	4	2	4	12	4	1

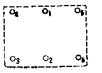
		Arrangement in Σ, *i.e.* 								Values of g, M, N, U, V, S, U' and V' in Eq. (V.3)								g
		σ_1	σ_2	σ_3	σ_4	σ_5	σ_6	σ_7	σ_8	g	M	N	U	V	S	U'	V'	
$\mathfrak{D}C^{\pm}_{\sigma^{\pm}(\pm)}$	$\mathfrak{D}C_{\Sigma\{\sigma^{\pm}(\pm),6\sigma(0)\}}$	$[\pm]$								0	0	0	0	0	0	0	0	1
	$\mathfrak{D}C_{\Sigma\{\sigma^{\pm}(\pm),6\sigma(H)\}}$	$[\pm]$					●			1	0	1	0	0	2	1	0	2
		$[\pm]$						●		1	1	0	0	0	2	0	1	4

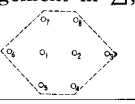
$\mathfrak{Q}C^{\pm}_{\sigma^{\pm}(\pm)}$	$\mathfrak{Q}C_{\sum\{\sigma^{\pm}(\pm),6\sigma(2H)\}}$	[$\pm$]	●				●	●		2	1	1	0	1	4	1	1	4
		[$\pm$]					●		●	2	1	1	0	0	4	1	1	4
		[$\pm$]	●				●			2	0	2	0	0	4	2	0	1
		[$\pm$]						●	●	2	2	0	1	0	4	0	2	2
		[$\pm$]		●				●		2	2	0	0	0	4	0	2	2
		[$\pm$]			●			●		2	2	0	0	0	4	0	2	2
	$\mathfrak{Q}C_{\sum\{\sigma^{\pm}(\pm),6\sigma(3H)\}}$	[$\pm$]				●	●	●	●	3	2	1	1	1	6	1	2	4
		[$\pm$]	●				●	●		3	1	2	0	1	6	2	1	4
		[$\pm$]		●			●	●		3	2	1	0	1	6	1	2	4
		[$\pm$]			●	●	●	●		3	2	1	0	2	6	1	2	2
		[$\pm$]		●			●		●	3	2	1	0	0	6	1	2	2
		[$\pm$]		●				●	●	3	3	0	1	0	6	0	3	4
	$\mathfrak{Q}C_{\sum\{\sigma^{\pm}(\pm),6\sigma(4H)\}}$	[$\pm$]	●			●	●	●		4	2	2	1	2	8	2	2	2
		[$\pm$]		●			●	●	●	4	3	1	1	1	8	1	3	4
		[$\pm$]			●	●	●	●	●	4	3	1	1	2	8	1	3	4
		[$\pm$]	●	●		●	●			4	2	2	0	2	8	2	2	2
		[$\pm$]	●		●	●	●			4	2	2	0	2	8	2	2	2
		[$\pm$]		●	●			●	●	4	4	0	2	0	8	0	4	1
	$\mathfrak{Q}C_{\sum\{\sigma^{\pm}(\pm),6\sigma(5H)\}}$	[$\pm$]	●	●		●	●	●		5	3	2	1	3	10	2	3	4
		[$\pm$]		●	●	●	●	●		5	4	1	2	2	10	1	4	2
	$\mathfrak{Q}C_{\sum\{\sigma^{\pm}(\pm),6\sigma(6H)\}}$	[$\pm$]	●	●	●	●	●	●		6	4	2	2	4	12	2	4	1

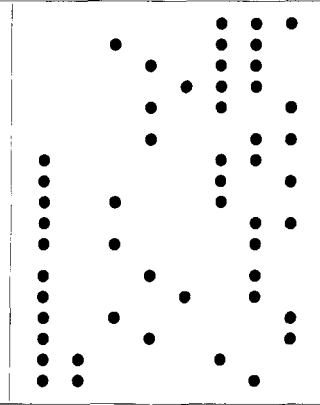
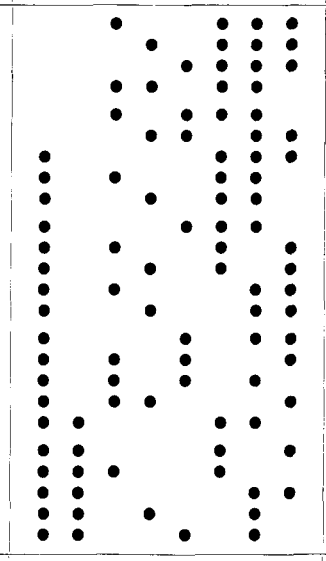
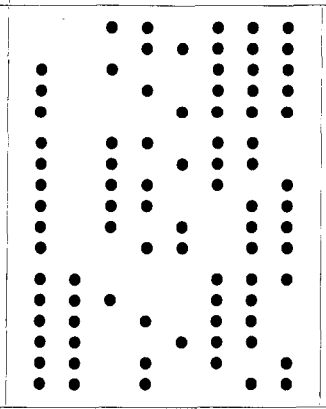
		Arrangement in $\sum$, *i. e.* 										Values of g, M, N, U, W, T, U', V' and W' in Eq. (V. 3)									g
		σ_1	σ_2	σ_3	σ_4	σ_5	σ_6	σ_7	σ_8	σ_9	σ_{10}	g	M	N	U	W	T	U'	V'	W'	
$\mathfrak{Q}C^{\pm}_{\sigma^{\pm}(\pm)}$	$\mathfrak{Q}C_{\sum\{\sigma^{\pm}(\pm),8\sigma(0)\}}$	[$\pm$]										0	0	0	0	0	0	0	0	0	1
	$\mathfrak{Q}C_{\sum\{\sigma^{\pm}(\pm),8\sigma(H)\}}$	[$\pm$]						●				1	0	1	0	0	4	1	0	0	2
		[$\pm$]							●			1	0	1	0	0	4	0	1	0	4
		[$\pm$]								●		1	1	0	0	0	3	0	0	1	2
	$\mathfrak{Q}C_{\sum\{\sigma^{\pm}(\pm),8\sigma(2H)\}}$	[$\pm$]						●	●			2	0	2	1	0	8	1	1	0	4
		[$\pm$]						●		●		2	1	1	0	1	7	1	0	1	4
		[$\pm$]						●			●	2	0	2	0	0	8	1	1	0	4
		[$\pm$]	●					●				2	0	2	0	0	8	2	0	0	1
		[$\pm$]							●	●		2	1	1	1	0	7	0	1	1	4
		[$\pm$]							●		●	2	0	2	0	0	8	0	2	0	2
		[$\pm$]		●					●			2	0	2	0	0	8	0	2	0	2
		[$\pm$]			●				●			2	1	1	0	0	7	0	1	1	4
		[$\pm$]				●			●			2	0	2	0	1	8	0	2	0	2
		[$\pm$]			●					●		2	2	0	0	1	6	0	0	2	1
	$\mathfrak{Q}C_{\sum\{\sigma^{\pm}(\pm),8\sigma(3H)\}}$	[$\pm$]						●	●	●		3	1	2	2	1	11	1	1	1	4
		[$\pm$]						●	●		●	3	0	3	1	0	12	1	2	0	4
		[$\pm$]	●					●	●			3	0	3	1	0	12	2	1	0	4
		[$\pm$]		●				●	●			3	0	3	1	0	12	1	2	0	4
		[$\pm$]			●			●	●			3	1	2	1	1	11	1	1	1	4
		[$\pm$]				●		●	●			3	0	3	2	1	12	1	2	0	2
		[$\pm$]						●		●	●	3	1	2	1	1	11	1	1	1	4
		[$\pm$]	●					●		●		3	1	2	0	2	11	2	0	1	2
		[$\pm$]		●				●		●		3	1	2	0	1	11	1	1	1	4
		[$\pm$]			●			●		●		3	2	1	0	3	10	1	0	2	2
		[$\pm$]		●				●			●	3	0	3	0	1	12	1	2	0	2
		[$\pm$]							●	●	●	3	1	2	2	0	11	0	2	1	2
		[$\pm$]		●					●	●		3	1	2	1	0	11	0	2	1	4

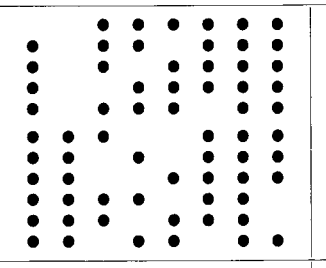
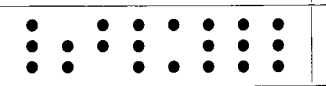
$\Sigma C^{\ddagger}_{\sigma^{\ddagger}(\ddagger)}$	$\Sigma C_{\Sigma\{\sigma^{\ddagger}(\ddagger),8\sigma(3H)\}}$	[‡]	●		●			●	●		3	2	1	1	1	10	0	1	2	4
		[‡]				●		●	●		3	1	2	1	1	11	0	2	1	4
		[‡]		●				●		●	3	0	3	0	1	12	0	3	0	4
		[‡]			●			●		●	3	1	2	0	0	11	0	2	1	2
	$\Sigma C_{\Sigma\{\sigma^{\ddagger}(\ddagger),8\sigma(4H)\}}$	[‡]				●	●	●	●		4	1	3	3	1	15	1	2	1	4
		[‡]	●			●	●	●			4	1	3	2	2	15	2	1	1	4
		[‡]		●		●	●	●			4	1	3	2	1	15	1	2	1	4
		[‡]			●	●	●	●			4	2	2	2	3	14	1	1	2	4
		[‡]				●	●	●	●		4	1	3	3	2	15	1	2	1	4
		[‡]	●			●	●			●	4	0	4	2	0	16	2	2	0	2
		[‡]		●		●	●			●	4	0	4	1	1	16	1	3	0	4
		[‡]			●	●	●			●	4	1	3	1	1	15	1	2	1	4
		[‡]				●	●	●		●	4	0	4	2	1	16	1	3	0	4
		[‡]	●	●		●	●				4	0	4	2	0	16	2	2	0	2
		[‡]	●		●	●	●				4	1	3	1	2	15	2	1	1	4
		[‡]	●			●	●				4	0	4	2	1	16	2	2	0	2
		[‡]		●	●	●	●				4	1	3	2	1	15	1	2	1	4
		[‡]		●		●		●	●		4	1	3	1	2	15	1	2	1	4
		[‡]			●	●		●	●		4	2	2	1	3	14	1	1	2	4
		[‡]	●		●	●		●			4	2	2	0	5	14	2	0	2	1
		[‡]		●			●	●	●		4	1	3	2	1	15	0	3	1	4
		[‡]			●		●	●	●		4	2	2	2	1	14	0	2	2	2
		[‡]		●	●		●	●			4	2	2	2	1	14	0	2	2	2
		[‡]		●		●	●	●			4	1	3	1	1	15	0	3	1	4
		[‡]			●	●	●	●			4	2	2	2	2	14	0	2	2	2
		[‡]		●		●	●			●	4	0	4	0	2	16	0	4	0	1
	$\Sigma C_{\Sigma\{\sigma^{\ddagger}(\ddagger),8\sigma(5H)\}}$	[‡]	●				●	●	●	●	5	1	4	4	2	19	2	2	1	2
		[‡]		●			●	●	●	●	5	1	4	3	2	19	1	3	1	4
		[‡]			●		●	●	●	●	5	2	3	3	3	18	1	2	2	4
		[‡]				●	●	●	●	●	5	1	4	4	2	19	1	3	1	4
		[‡]	●	●			●	●	●		5	1	4	3	2	19	2	2	1	4
		[‡]	●		●		●	●	●		5	2	3	2	5	18	2	1	2	4
		[‡]	●			●	●	●	●		5	1	4	3	3	19	2	2	1	4
		[‡]		●	●		●	●	●		5	2	3	3	3	18	1	2	2	4
		[‡]		●		●	●	●	●		5	1	4	3	2	19	1	3	1	4
		[‡]			●	●	●	●	●		5	2	3	4	4	18	1	2	2	2
		[‡]	●	●			●	●		●	5	0	5	3	1	20	2	3	0	4
		[‡]	●		●		●	●		●	5	1	4	2	2	19	2	2	1	2
		[‡]		●	●		●	●		●	5	1	4	2	2	19	1	3	1	4
		[‡]		●		●	●	●		●	5	0	5	2	2	20	1	4	0	2
		[‡]		●	●		●		●	●	5	2	3	2	4	18	1	2	2	2
		[‡]		●	●			●	●	●	5	2	3	3	2	18	0	3	2	4
		[‡]		●		●		●	●	●	5	1	4	2	2	19	0	4	1	2
	$\Sigma C_{\Sigma\{\sigma^{\ddagger}(\ddagger),8\sigma(6H)\}}$	[‡]	●	●			●	●	●	●	6	1	5	5	3	23	2	3	1	4
		[‡]	●		●		●	●	●	●	6	2	4	4	5	22	2	2	2	2
		[‡]		●	●		●	●	●	●	6	2	4	4	4	22	1	3	2	4
		[‡]		●		●	●	●	●	●	6	1	5	4	3	23	1	4	1	4
		[‡]			●	●	●	●	●	●	6	2	4	5	4	22	1	3	2	4
		[‡]	●	●	●		●	●	●		6	2	4	4	5	22	2	2	2	2
		[‡]	●	●		●	●	●	●		6	1	5	4	3	23	2	3	1	4
		[‡]	●		●	●	●	●			6	2	4	4	6	22	2	2	2	2
		[‡]	●	●		●	●			●	6	0	6	4	2	24	2	4	0	1
		[‡]		●	●	●		●	●	●	6	2	4	4	3	22	0	4	2	1
	$\Sigma C_{\Sigma\{\sigma^{\ddagger}(\ddagger),8\sigma(7H)\}}$	[‡]	●	●	●		●	●	●	●	7	2	5	6	6	26	2	3	2	4
		[‡]	●	●		●	●	●	●	●	7	1	6	6	4	27	2	4	1	2
		[‡]	●	●	●	●		●	●	●	7	2	5	6	5	26	1	4	2	2
	$\Sigma C_{\Sigma\{\sigma^{\ddagger}(\ddagger),8\sigma(8H)\}}$	[‡]	●	●	●	●	●	●	●	●	8	2	6	8	7	30	2	4	2	1

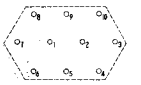
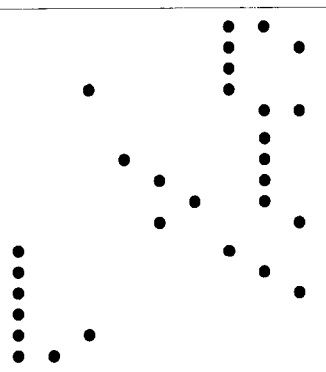
TABLE V. ΩC's on (110)–, (100)– and (111)–lattice planes

		Arrangement in Σ, *i. e.* 						Values of g, L, U, V, W, S and T in Eq. (V. 6)							g
		σ_1	σ_2	σ_3	σ_4	σ_5	σ_6	g	L	U	V	W	S	T	
ΩC	$\Omega C_{\Sigma(0)}$							0	0	0	0	0	0	0	1
	$\Omega C_{\Sigma\{6\sigma(\mathrm{H})\}}$	●						1	0	0	0	6	1	2	2
				●				1	0	0	0	0	1	3	4
	$\Omega C_{\Sigma\{6\sigma(2\mathrm{H})\}}$	●	●					2	0	0	1	0	2	4	1
		●			●			2	1	0	0	1	2	5	4
					●	●		2	2	0	0	0	2	6	4
			●		●			2	1	0	0	1	2	5	4
				●	●			2	2	0	1	0	2	6	2
	$\Omega C_{\Sigma\{6\sigma(3\mathrm{H})\}}$	●		●	●			3	2	1	1	1	3	8	4
				●	●	●		3	3	0	1	0	3	9	4
			●		●		●	3	2	1	0	1	3	8	4
		●	●		●			3	1	1	1	1	3	7	4
			●		●	●		3	2	0	0	2	3	8	2
		●			●	●		3	2	2	0	0	3	8	2
	$\Omega C_{\Sigma\{6\sigma(4\mathrm{H})\}}$		●	●			●	4	3	2	1	1	4	11	4
		●	●	●			●	4	2	2	1	2	4	10	4
		●		●		●	●	4	3	1	1	2	4	11	4
		●	●			●	●	4	2	2	2	2	4	10	2
				●	●	●	●	4	4	0	2	0	4	12	1
	$\Omega C_{\Sigma\{6\sigma(5\mathrm{H})\}}$		●	●	●	●	●	5	4	2	2	2	5	14	2
		●	●	●		●	●	5	3	3	2	3	5	13	4
	$\Omega C_{\Sigma\{6\sigma(6\mathrm{H})\}}$	●	●	●	●	●	●	6	4	4	3	4	6	16	1

		Arrangement in Σ, *i. e.* 								Values of g, M, N, U, V and S in Eq. (V. 6)						g
		σ_1	σ_2	σ_3	σ_4	σ_5	σ_6	σ_7	σ_8	g	M	N	U	V	S	
ΩC	$\Omega C_{\Sigma(0)}$									0	0	0	0	0	0	1
	$\Omega C_{\Sigma\{8\sigma(\mathrm{H})\}}$						●			1	0	1	0	0	2	2
								●		1	1	0	0	0	2	4
		●								1	0	0	0	0	2	2
	$\Omega C_{\Sigma\{8\sigma(2\mathrm{H})\}}$						●	●		2	1	1	0	1	4	4
							●		●	2	1	1	0	0	4	4
				●			●			2	0	2	0	0	4	1
								●	●	2	2	0	1	0	4	2
					●			●		2	2	0	0	0	4	2
						●		●		2	2	0	0	0	4	2
		●					●			2	0	1	1	0	4	2
		●						●		2	1	0	1	0	4	4
		●							●	2	1	0	0	1	4	4
		●		●						2	0	1	0	0	4	2
		●	●							2	0	0	1	0	4	1

$\Sigma C_{\Sigma\{8\sigma(3H)\}}$		3	2	1	1	1	6	4
		3	1	2	0	1	6	4
		3	2	1	0	1	6	4
		3	2	1	0	2	6	2
		3	2	1	0	0	6	2
		3	3	0	1	0	6	4
		3	1	1	2	1	6	4
		3	1	1	1	1	6	4
		3	0	2	1	0	6	2
		3	2	0	2	1	6	4
		3	1	1	1	0	6	4
		3	2	0	1	1	6	4
		3	2	0	2	0	6	2
		3	1	1	0	2	6	4
		3	2	0	0	2	6	2
		3	0	1	2	0	6	2
		3	1	0	2	1	6	4
ΣC $\Sigma C_{\Sigma\{8\sigma(4H)\}}$		4	2	2	1	2	8	2
		4	3	1	1	1	8	4
		4	3	1	1	2	8	4
		4	2	2	0	2	8	2
		4	2	2	0	2	8	2
		4	4	0	2	0	8	1
		4	2	1	3	2	8	4
		4	1	2	2	1	8	4
		4	2	1	2	2	8	4
		4	2	1	3	2	8	2
		4	1	2	1	2	8	4
		4	2	1	1	2	8	2
		4	2	1	2	2	8	4
		4	3	0	2	2	8	4
		4	3	0	3	1	8	4
		4	2	1	1	2	8	4
		4	2	1	2	0	8	2
		4	2	1	0	4	8	2
		4	1	1	3	2	8	4
		4	1	1	3	1	8	4
		4	0	2	3	0	8	1
		4	2	0	4	2	8	2
		4	2	0	3	2	8	2
		4	2	0	3	2	8	2
$\Sigma C_{\Sigma\{8\sigma(5H)\}}$		5	3	2	1	3	10	4
		5	4	1	2	2	10	2
		5	2	2	3	3	10	4
		5	3	1	3	3	10	4
		5	3	1	4	3	10	4
		5	2	2	2	3	10	4
		5	2	2	3	2	10	2
		5	2	2	1	4	10	2
		5	3	1	2	4	10	4
		5	3	1	3	2	10	4
		5	4	0	4	2	10	2
		5	2	1	5	3	10	4
		5	1	2	4	2	10	4
		5	2	1	4	3	10	4
		5	2	1	4	4	10	2
		5	2	1	4	2	10	2
		5	3	0	5	3	10	4

$\mathfrak{D}C$	$\mathfrak{D}C_{\Sigma\{8\sigma(6H)\}}$		6	4	2	2	4	12	1
			6	3	2	3	5	12	4
			6	3	2	4	4	12	4
			6	4	1	5	4	12	2
			6	4	1	4	4	12	2
			6	2	2	6	4	12	2
			6	3	1	6	4	12	4
			6	3	1	6	5	12	4
			6	2	2	5	4	12	2
			6	2	2	5	4	12	2
			6	4	0	7	4	12	1
	$\mathfrak{D}C_{\Sigma\{8\sigma(7H)\}}$		7	4	2	5	6	14	2
			7	3	2	7	6	14	4
			7	4	1	8	6	14	2
	$\mathfrak{D}C_{\Sigma\{8\sigma(8H)\}}$		8	4	2	9	8	16	1

		Arrangement in Σ, *i. e.* 	Values of g, M, N, U, W and T in Eq. (V. 6)						$\boldsymbol{g}$
		σ_1 σ_2 σ_3 σ_4 σ_5 σ_6 σ_7 σ_8 σ_9 σ_{10}	g	M	N	U	W	T	
$\mathfrak{D}C$	$\mathfrak{D}C_{\Sigma(0)}$		0	0	0	0	0	0	1
	$\mathfrak{D}C_{\Sigma\{10\sigma(H)\}}$		1	0	1	0	0	4	6
			1	1	0	0	0	3	2
			1	0	0	0	0	4	2
	$\mathfrak{D}C_{\Sigma\{10\sigma(2H)\}}$		2	0	2	1	0	8	4
			2	1	1	0	1	7	4
			2	0	2	0	0	8	4
			2	0	2	0	0	8	1
			2	1	1	1	0	7	4
			2	0	2	0	0	8	2
			2	0	2	0	0	8	2
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			2	0	2	0	1	8	2
			2	2	0	0	1	6	1
			2	0	1	1	0	8	2
			2	0	1	1	0	8	4
			2	1	0	1	0	7	4
			2	0	1	0	1	8	4
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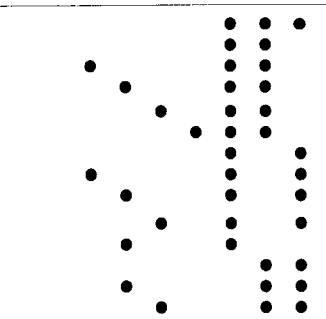
	$\mathfrak{D}C_{\Sigma\{10\sigma(3H)\}}$		3	1	2	2	1	11	4
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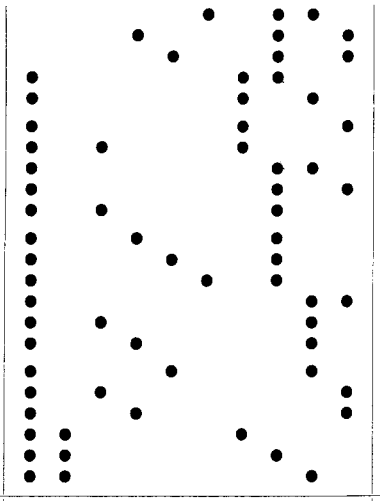
			3	0	3	1	0	12	4
			3	0	3	1	0	12	4
			3	1	2	1	1	11	4
			3	0	3	2	1	12	2
			3	1	2	1	1	11	4
			3	1	2	0	2	11	2
			3	1	2	0	1	11	4
			3	2	1	0	3	10	2
			3	0	3	0	1	12	2
			3	1	2	2	0	11	2
			3	1	2	1	0	11	4
			3	2	1	1	1	10	4

$\mathfrak{Q}C_{\sum\{10\sigma(3H)\}}$		3	1	2	1	1	11	4
		3	0	3	0	1	12	4
		3	1	2	0	0	11	2
		3	0	2	3	0	12	4
		3	1	1	2	1	11	4
		3	0	2	1	1	12	4
		3	0	2	1	0	12	2
		3	1	1	3	0	11	4
		3	0	2	1	1	12	4
		3	0	2	1	0	12	4
		3	0	2	1	1	12	4
		3	1	1	2	0	11	4
		3	0	2	2	1	12	2
		3	1	1	2	1	11	4
		3	1	1	1	1	11	4
		3	1	1	1	1	11	4
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		3	0	2	1	1	12	4
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		3	0	1	2	0	12	2
		3	0	1	2	1	12	4
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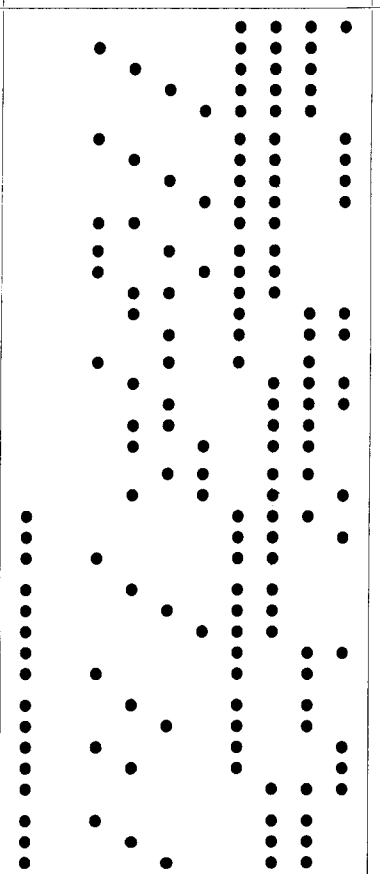
$\mathfrak{Q}C$								
$\mathfrak{Q}C_{\sum\{10\sigma(4H)\}}$		4	1	3	3	1	15	4
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		4	1	3	3	2	15	4
		4	0	4	2	0	16	2
		4	0	4	1	1	16	4
		4	1	3	1	1	15	4
		4	0	4	2	1	16	4
		4	0	4	2	0	16	2
		4	1	3	1	2	15	4
		4	0	4	2	1	16	2
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		4	2	2	2	2	14	2
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		4	1	2	4	1	15	4
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		4	1	2	2	2	15	4
		4	1	2	2	2	15	4
		4	2	1	3	3	14	2
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		4	1	2	4	1	15	4
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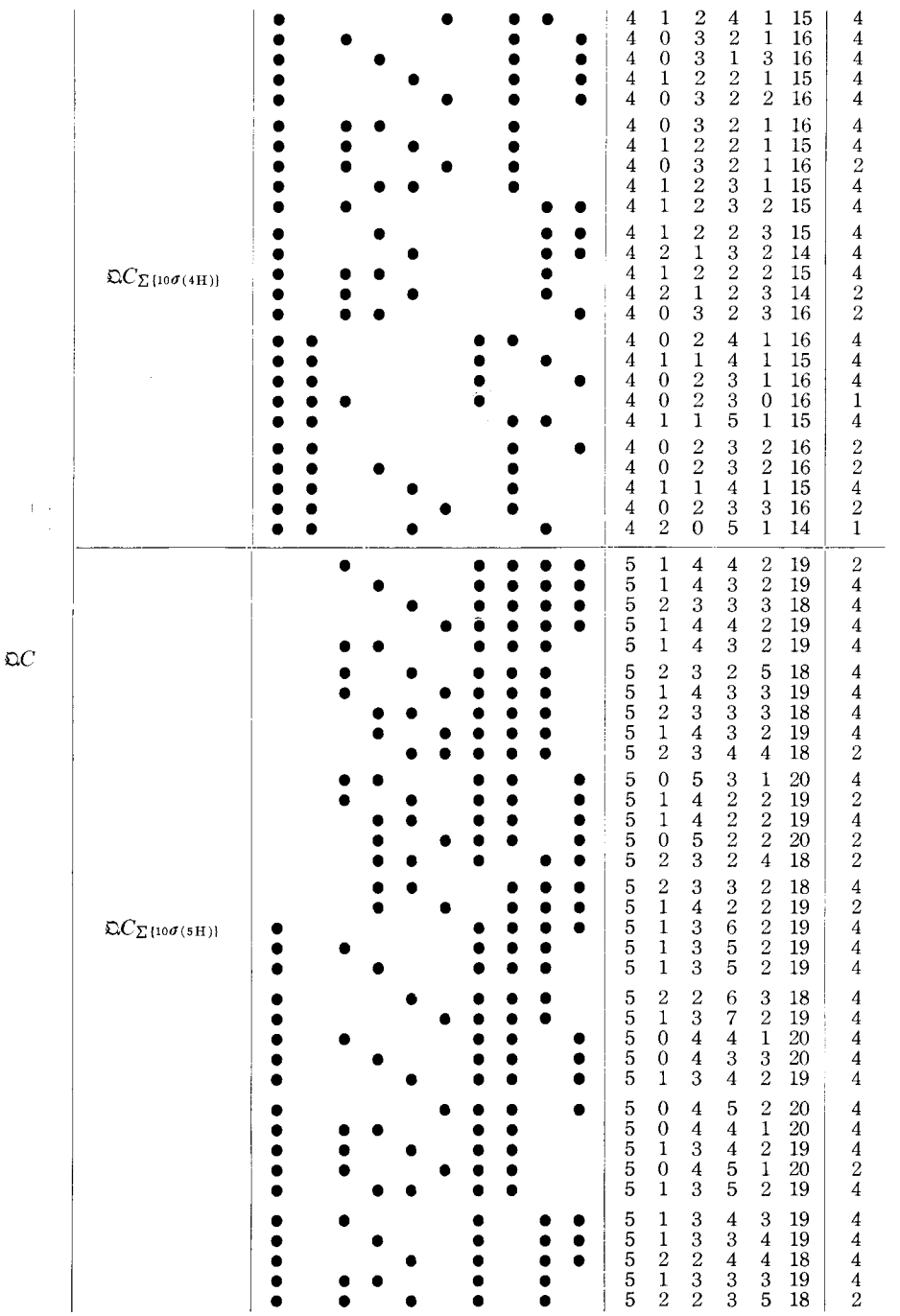

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4	1	2	2	1	15	4
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5	0	4	5	2	20	4
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5	1	3	3	4	19	4
5	2	2	4	4	18	4
5	1	3	3	3	19	4
5	2	2	3	5	18	2

ΣC

$\Sigma C_{\Sigma\{10\sigma(5H)\}}$	●		●	●			●			●	5	0	4	3	3	20	2
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	●				●			●	●	●	5	2	2	5	2	18	4
	●					●		●	●	●	5	1	3	5	2	19	4
	●		●	●				●	●		5	1	3	4	2	19	4
	●		●		●			●	●		5	2	2	4	3	18	4
	●		●			●		●	●		5	1	3	4	2	19	4
	●			●	●			●	●		5	2	2	5	2	18	4
	●			●		●		●	●		5	1	3	4	2	19	4
	●				●	●		●	●		5	2	2	6	2	18	2
	●		●	●				●		●	5	0	4	3	3	20	4
	●		●		●			●		●	5	1	3	3	2	19	4
	●		●			●		●		●	5	0	4	3	2	20	4
	●			●	●			●		●	5	1	3	3	3	19	4
	●			●		●		●		●	5	0	4	2	4	20	2
	●		●	●	●			●			5	1	3	4	2	19	4
	●		●	●					●	●	5	1	3	4	4	19	4
	●		●		●				●	●	5	2	2	4	4	18	4
	●			●	●				●	●	5	2	2	4	4	18	2
	●	●				●	●	●			5	1	2	7	2	19	4
	●	●				●	●			●	5	0	3	5	2	20	4
	●	●	●			●	●				5	0	3	5	1	20	4
	●	●		●		●	●				5	0	3	5	2	20	4
	●	●			●	●	●				5	1	2	6	2	19	4
	●	●				●	●				5	0	3	6	3	20	2
	●	●				●			●	●	5	1	2	6	2	19	4
	●	●	●			●			●		5	1	2	5	2	19	2
	●	●		●		●			●		5	1	2	5	2	19	4
	●	●			●	●			●		5	2	1	6	3	18	2
	●	●		●		●				●	5	0	3	4	3	20	2
	●	●					●	●	●	●	5	1	2	7	2	19	2
	●	●		●			●	●			5	1	2	6	2	19	4
	●	●			●		●	●			5	2	1	7	2	18	4
	●	●				●	●	●			5	1	2	6	3	19	4
	●	●		●			●			●	5	0	3	4	4	20	4
	●	●			●		●			●	5	1	2	5	2	19	2
$\Sigma C_{\Sigma\{10\sigma(6H)\}}$			●	●			●	●	●	●	6	1	5	5	3	23	4
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				●	●		●	●	●	●	6	2	4	4	4	22	4
				●		●	●	●	●	●	6	1	5	4	3	23	4
					●	●	●	●	●	●	6	2	4	5	4	22	4
			●	●	●		●	●	●		6	2	4	4	5	22	2
			●	●		●	●	●	●		6	1	5	4	3	23	4
			●		●	●	●	●	●		6	2	4	4	6	22	2
			●	●		●	●	●		●	6	0	6	4	2	24	1
				●	●	●		●	●	●	6	2	4	4	3	22	1
	●		●				●	●	●	●	6	1	4	7	3	23	4
	●			●			●	●	●	●	6	1	4	6	4	23	4
	●				●		●	●	●	●	6	2	3	7	4	22	4
	●					●	●	●	●	●	6	1	4	8	3	23	4
	●		●	●			●	●	●		6	1	4	6	3	23	4
	●		●		●		●	●	●		6	2	3	6	5	22	4
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	●		●	●			●	●		●	6	0	5	5	3	24	4
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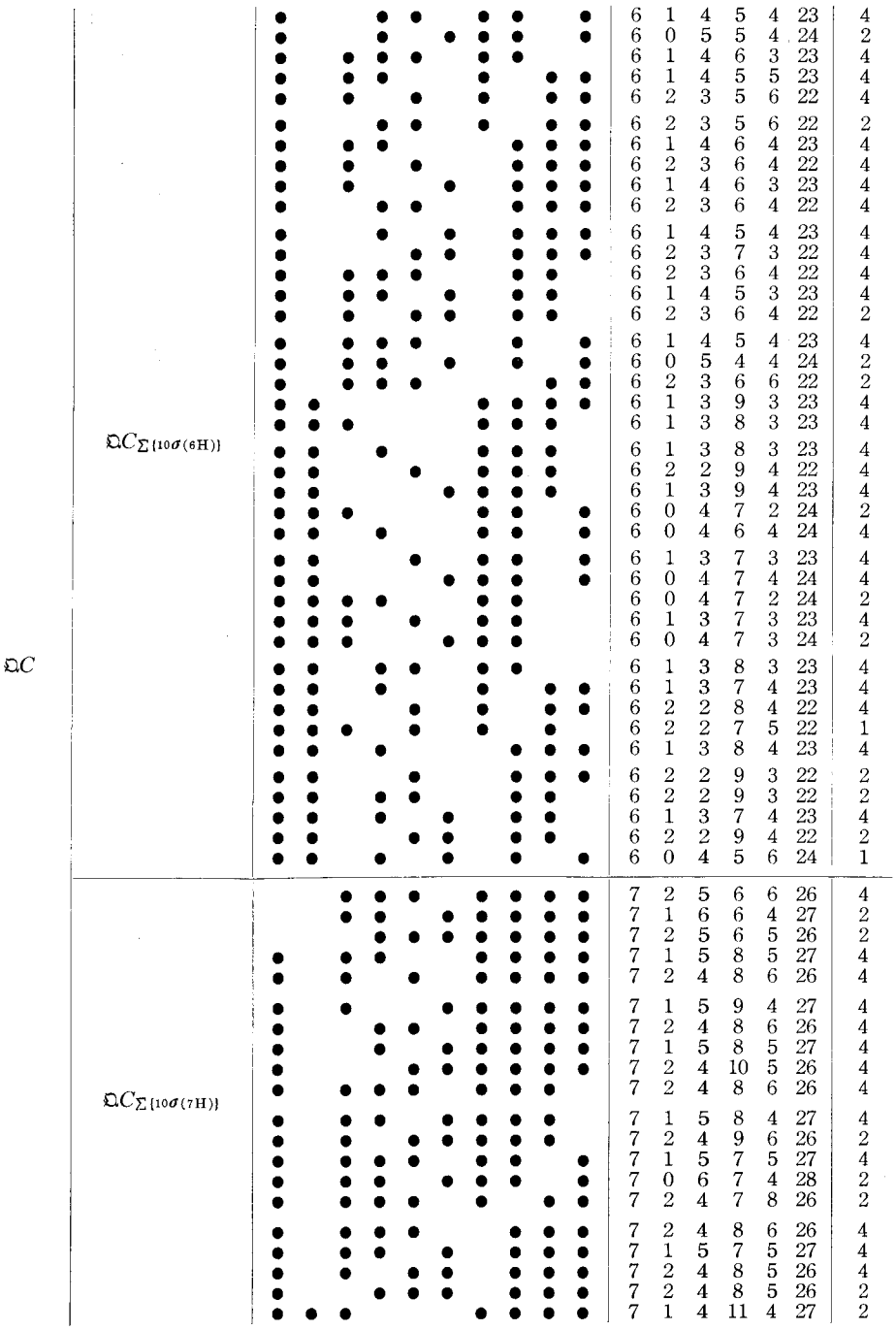
ΩC
ΩC∑{10σ(6H)}
ΩC∑{10σ(7H)}

ΣC	$\Sigma C_{\Sigma\{10\sigma(7H)\}}$	●	●		●			●	●	●	●	7	1	4	10	5	27	4
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		●	●				●	●	●	●	●	7	1	4	11	5	27	4
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		●	●	●		●		●	●	●		7	2	3	10	6	26	4
		●	●	●			●	●	●	●		7	1	4	10	5	27	4
		●	●		●		●	●	●	●		7	1	4	10	5	27	4
		●	●			●	●	●	●	●		7	2	3	12	6	26	2
		●	●	●	●			●	●		●	7	0	5	9	4	28	4
		●	●	●		●		●	●		●	7	1	4	9	4	27	2
		●	●		●	●		●	●		●	7	1	4	9	5	27	4
		●	●		●		●	●	●		●	7	0	5	8	6	28	2
		●	●		●	●		●		●	●	7	2	3	10	6	26	2
		●	●			●	●	●		●	●	7	2	3	11	5	26	4
		●	●		●	●			●	●	●	7	2	3	11	5	26	4
		●	●		●		●		●	●	●	7	1	4	9	6	27	2
	$\Sigma C_{\Sigma\{10\sigma(8H)\}}$			●	●	●	●	●	●	●	●	8	2	6	8	7	30	1
		●		●	●	●		●	●	●	●	8	2	5	10	8	30	4
		●		●	●		●	●	●	●	●	8	1	6	10	6	31	4
		●		●		●	●	●	●	●	●	8	2	5	11	7	30	4
		●			●	●	●	●	●	●	●	8	2	5	11	7	30	2
		●		●	●	●	●		●	●	●	8	2	5	10	7	30	2
		●	●	●	●			●	●	●	●	8	1	5	13	6	31	4
		●	●	●		●		●	●	●	●	8	2	4	13	7	30	2
		●	●		●	●		●	●	●	●	8	2	4	13	7	30	4
		●	●		●		●	●	●	●	●	8	1	5	12	7	31	4
		●	●			●	●	●	●	●	●	8	2	4	14	7	30	4
		●	●	●	●	●		●	●	●		8	2	4	13	7	30	2
		●	●	●	●		●	●	●	●		8	1	5	12	6	31	4
		●	●	●		●	●	●	●	●		8	2	4	13	8	30	2
		●	●	●	●		●	●	●		●	8	0	6	11	6	32	1
		●	●		●	●	●		●	●	●	8	2	4	13	7	30	1
	$\Sigma C_{\Sigma\{10\sigma(9H)\}}$	●		●	●	●	●	●	●	●	●	9	2	6	13	9	34	2
		●	●	●	●	●		●	●	●	●	9	2	5	16	9	34	4
		●	●	●	●		●	●	●	●	●	9	1	6	15	8	35	2
		●	●		●	●	●	●	●	●	●	9	2	5	16	9	34	2
	$\Sigma C_{\Sigma\{10\sigma(10H)\}}$	●	●	●	●	●	●	●	●	●	●	10	2	6	19	11	38	1