Spectral line broadening of atoms by noble gases

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Abstract. The complex universal approach for calculations of the binary broadening of atomic
spectral lines by buffer noble gas atoms is presented. The interatomic interaction is described
on the basis of the Buckingham potential, parameterized with the help of ab initio electron
modeling. The Unified Frank-Condon Theory is used for the calculations of the total line
profile. For the first time the impact limit is determined exactly using the Van der Waals long-
range tail of the potential and taking into account the degeneracy of quasimolecular states but
neglecting non-adiabatic effects. The general asymptotic wings dependences of the profile are
established for the Buckingham parameterized potential. The receipts of the wings cut-offs are
formulated for the approximate but sufficiently accurate evaluation of the total line profile
using only the Van der Waals part of potential to be applied in large scale calculations of
radiative transfer.

1. The impact Van der Waals broadening with account of degeneracy

The impact width of the spectral line corresponding to the dipole transition of the compound system of
the radiator atom A and buffer gas atom X is related to the elements of scattering matrix, expressed in
the form (compare with [1])

\[
\sigma_{iJjJ}^{(l)}(\epsilon_i) = \text{Re} \left[ \frac{\pi}{k^2} \sum_{J,J'} \sum_{J''} \sum_{J'''} (-1)^{l-J-J'} (2J+1)(2J'+1) \left\{ \begin{array}{ccc} J & J & 1 \\ J & J & I \end{array} \right\} \left\{ \begin{array}{ccc} J' & J' & 1 \\ J' & J' & J'' \end{array} \right\} \delta_{J'-J''} \cdot S_{J,J'}(\epsilon_i) \right].
\]

(1)

Here \( \hbar \), \( \hbar' \) are total (electronic + nuclear) angular momenta of the diatom A–X, \( \hbar_l, \hbar'_l \) are angular momenta of the relative motion of A and X, \( k \) is the wave number of the relative motion of A and X at
infinite separation, \( S_{J,J'}(\epsilon_i) \) and \( S_{J,J'}^{\gamma\gamma'}(\epsilon_i) \) are scattering matrix elements for A(\( \gamma_l \))–X and
A(\( \gamma'_l \))–X collisions at relative kinetic energy \( \epsilon_i = \hbar^2 k^2 / 2\mu \), \( \mu \) is the A–X reduced mass, \( \gamma \) stands for
the corresponding sets of quantum numbers for the initial i and final states f of A, while the curly
brackets designate 6-j symbols [2]. Since the impact broadening corresponds to elastic distant
collisions the main contribution to the above sum is given by \( \mathbf{J}_i, \mathbf{J}_f \gg 1 \). At the same time \( \hat{\mathbf{J}}_i, \hat{\mathbf{J}}_f \sim 1 \) as mostly lower excited levels are of importance for problem under consideration. Then \( \mathbf{I}, \mathbf{I}' \) may differ from \( \mathbf{J}_i, \mathbf{J}_f \) by the value of the order of 1, and the difference between \( \mathbf{J}_i \) and \( \mathbf{J}_f \) is also of the order of 1. Keeping this in mind it is suitable to introduce the new summation variables \( J = (\mathbf{J}_i + \mathbf{J}_f)/2, \rho = J_i - J_f, m = J_i - \ell, m' = J_f - \ell \). As \( \mathbf{J} \gg 1 \) the asymptotic of \( 6\mathbf{j} \) symbols could be used (see, e.g. [3]), and the expression for the broadening cross section \( \sigma_{\nu \mathbf{I};\nu \mathbf{I}'(\mathbf{J}_i)}^{(1)}(\varepsilon_i) \) could be simplified as follows

\[
\sigma_{\nu \mathbf{I};\nu \mathbf{I}'(\mathbf{J}_i)}^{(1)}(\varepsilon_i) = \text{Re} \left\{ \frac{\pi}{k^2} \sum_{\nu} 2J \sum_{m,m'} \left[ \frac{1}{3} \sum_{\nu} (-1)^{\nu - \nu'} \left[ \frac{J_i}{m} \frac{J_f}{m'} \right] \right] \right\}
\]

\[
\left[ \delta_{\nu \nu'} - e^{i\nu \mu} S_{\nu \nu'}^{J_i(\nu \nu')} (\varepsilon_i) S_{\nu' \nu}^{J_f(\nu \nu')} (\varepsilon_f) \right],
\]

where square brackets designate \( 3\mathbf{j} \) symbols [2]. Since the distant collisions correspond to the Van der Waals tail of real potential, the matrix elements of interaction in the Hund case (c) could be represented in the collisions frame in the form

\[
\langle \nu m | \nu' (\mathbf{R}) | m', \nu' \rangle = -\frac{C_{\nu \nu'}^{(0,\mathbf{I})}}{R^\alpha} \left[ \delta_{\nu m} - B_{\nu \nu'}^{(2,\mathbf{I})} F(j,m,m') \right],
\]

\[
C_{\nu \nu'}^{(0,\mathbf{I})} = \frac{1}{\pi} \frac{1}{(2j+1)^{1/2}} \int_0^\infty \langle \nu | \alpha_{\mathbf{I}}^{(0)} (\omega) | \nu' \rangle \langle \nu' | S^2 | \nu \rangle d\omega,
\]

\[
B_{\nu \nu'}^{(2,\mathbf{I})} = \frac{\sqrt{2}}{2} \int_0^\infty \langle \nu | \alpha_{\mathbf{I}}^{(0)} (\omega) | \nu' \rangle \langle \nu' | S^2 | \nu \rangle d\omega,
\]

\[
F(j,m,m') = \sum_{\Omega \neq \cdots} D_j^{(\mathbf{I})} (0, \pi / 2, \pi) \text{Re} \left[ \frac{J}{\Omega} \frac{J}{\Omega} \right] D_m^{(\mathbf{I})} (0, \pi / 2, \pi),
\]

where \( \mathbf{R} \) is the \( \mathbf{A}-\mathbf{X} \) internuclear distance; \( \alpha_{\mathbf{I}}^{(0)} (\omega), \alpha_{\mathbf{I}}^{(2)} (\omega), \alpha_{\mathbf{I}}^{(0)} (\omega) \) are reduced components in the \{\mathbf{k}, \mathbf{q}\} representation of the irreducible tensor of dynamical polarizability of radiator atom \( \mathbf{A} \) and buffer gas atom \( \mathbf{X} \); \( D_j^{(\mathbf{I})} (\alpha, \beta, \gamma) \) are the Wigner rotation matrices [2]. The quantities \( \mathbf{h} \Omega, \mathbf{h} \Omega' \) are the projections of the atom \( \mathbf{A} \) electronic angular momentum upon the direction of the total (electronic + nuclear) angular momentum of the diatom \( \mathbf{A}-\mathbf{X} \), that is perpendicular to the collisions frame. Using semiclassical approximation and assuming rectilinear trajectories, it is possible to obtain analytical result

\[
\sigma_{\nu \mathbf{I};\nu \mathbf{I}'(\mathbf{J}_i)}^{(2)}(\varepsilon_i) = 2\pi \int_0^\infty db d\mathbf{b} \sum_{\mathbf{m},\mathbf{m}'} \left[ \frac{J_i}{m} \frac{J_f}{m'} \right] \left[ \frac{1}{2} \right] \left[ \frac{3\pi}{8\hbar^2} \right] \left[ \frac{C_{\nu \nu'}^{(0,\mathbf{I})}}{C_{\nu \nu'}^{(2,\gamma \gamma')}} \right] \left( \delta_{\nu \nu'} - \left( \frac{C_{\nu \nu'}^{(0,\mathbf{I})}}{C_{\nu \nu'}^{(2,\gamma \gamma')}} \right) F(j,m,m') \right],
\]

\[
\Gamma_{\mathbf{m},\mathbf{m}'}^{(0,\mathbf{I};\nu \mathbf{I}')/2} = 1 + \frac{1}{C_{\nu \nu'}^{(0,\mathbf{I})} - C_{\nu \nu'}^{(2,\gamma \gamma')}} \left[ \frac{C_{\nu \nu'}^{(0,\mathbf{I})} - C_{\nu \nu'}^{(0,\mathbf{I})}}{C_{\nu \nu'}^{(2,\gamma \gamma')}} \right] F(j,m,m') - C_{\nu \nu'}^{(0,\mathbf{I})} B_{\nu \nu'}^{(2,\gamma \gamma')} F(j,m,m').
\]
Here $<u>$ is the mean velocity, $n_X$ is the density of buffer gas atoms, $\Gamma(z)$ is the gamma function. The obtained result takes into account strong Coriolis coupling between degenerate quasimolecular states, but the non-diagonal matrix elements between different “m” are neglected. At large distances the Coriolis interaction is larger in absolute value than the splitting between different molecular terms, arising due to the Van der Waals interaction between $A(j)$ (with $j>0$ or $1/2$) and $X$. That is why the adiabatic approach to the description of Van der Waals broadening is quite adequate, as well as assumption of the rectilinear trajectories of relative $A$ and $X$ motion and implementation of the quasiclassical theory of atomic collisions (see [4]).

2. Parameterizing of modified Buckingham potential

The study of interatomic interactions showed that they are well approximated by modified Buckingham type of potentials [5]. These potentials have typical repulsive exponential short-range core and the attractive Van der Waals long-range tail

$$U_b(r) = A \exp(-\alpha r) - \frac{C_6}{(r^2 + r_0^2)^{3/2}}.$$

(11)

Although this approximation could not mimic all characteristics of the real potential curves, it possesses all main properties regarding the behavior of real potentials first of all at small and large interatomic distances. The parameters in (11) for the particular states of the radiator $A$ and the buffer gas atom $X$ could be found either experimentally or from the quantum chemical calculations (QCh). The value of $C_6$ could be calculated as well in more universal manner using the perturbation theory in molecular basis and confronted with the values given by QCh. As an illustration of this approach the QCh calculations were performed for the potential curves $X^2\Sigma_{1/2}$, $A^2\Pi_{1/2}$ and $B^2\Sigma_{1/2}$ of the Na-Xe system, and the parameters of modified Buckingham potential were retrieved [6]: $X^2\Sigma_{1/2}$, $A = 116.869$ eV, $\alpha = 1.654$ Å$^{-1}$, $C_6 = 946.502$ eVÅ$^6$, $r_0 = 1.504$ Å; $A^2\Pi_{3/2}$, $A = 3214.79$ eV, $\alpha = 3.185$ Å$^{-1}$, $C_6 = 22.774$ eVÅ$^6$, $r_0 = 1.960$ Å; $B^2\Sigma_{1/2}$, $A = 102.829$ eV, $\alpha = 1.256$ Å$^{-1}$, $C_6 = 3408.543$ eVÅ$^6$, $r_0 = 1.566$ Å. The comparison with experimental data and results of other calculations demonstrates that both could be accurately approximated by (11). The coincidence of retrieved from QCh calculations $C_6$ values with ones, obtained within the perturbation theory is also quite reasonable.

3. Total profile within Unified Frank-Condon Theory and wing asymptotic

Basing on the knowledge of parameterized Buckingham potential for the particular quasimolecular states, involved in the certain radiative transition of compound system $A-X$, and having in the pocket the result for the impact width, obtained in the previous section, it is possible to describe the total profile $F(\Delta \omega)$ of spectral line within Unified Frank-Condon Theory (UFCT) [7] in the binary approximation

$$F(\Delta \omega) = \frac{1}{\pi} \frac{\Phi(\Delta \omega)}{(\Delta \omega)^2 + (\Delta \omega_{1/2})^2}, \quad \Phi(\Delta \omega) = \sum_{if} g(i \rightarrow f) \Phi_{if}(\Delta \omega), \quad g(i \rightarrow f) = \frac{N(i \rightarrow f)}{N(i_A \rightarrow f_A)},$$

(12)

$$\Phi_{if}(\Delta \omega) = \pi n_X <u> \int_0^\infty \frac{e^{de}}{(k_B T)^2} \exp \left( - \frac{e}{k_B T} \right) \times 2b db G_{ef}(b, e, \Delta \omega)^2.$$
\[
G_{ij}(b,\varepsilon,\Delta\omega) = \frac{2}{\hbar^2} \int_0^{\infty} \! dt \ \Delta U_{ij} \left[ R(t,b,\varepsilon) \right] \cos \left[ \Delta \omega t - \eta_{ij}(t,b,\varepsilon) \right], \quad (14)
\]
\[
\eta_{ij}(t,b,\varepsilon) = \frac{1}{\hbar} \int_0^{t} \! \Delta U_{ij} \left[ R(t',b,\varepsilon) \right] dt', \quad \Delta U_{ij}(r) = U_i(r) - U_j(r). \quad (15)
\]

where \(\Delta\omega = (\omega - \omega_0)\), \(\omega_0\) is the frequency of transition in the free atom \(A\), \(\omega\) is the radiation frequency, \(G_{ij}(b,\varepsilon,\Delta\omega)\) is the reduced Frank-Condon factor, \(\eta_{ij}(t,b,\varepsilon)\) is the phase shift versus the relative \(A-X\) motion along the trajectory \(R(t,b,\varepsilon)\) with the initial kinetic energy \(\varepsilon_b\) and the impact parameter \(b\), \(T\) is the temperature, \(k_B\) is the Boltzmann constant. In (12) \(g(i \to f)\) stands for the statistical weight, and \(N(i \to f)_{AX}\) is the number of the allowed dipole transitions with \(\Delta\Omega = 0, \pm 1\) (\(\Omega\) is the projection of the quasi-molecular electronic angular momentum on internuclear axis) between quasi-molecular electronic states corresponding to the potential curves \(U_i(r)\), and \(U_j(r)\), while \(N(i \to f)_{AX}\) is the total number of the allowed dipole transitions \(i \to f\) with \(m_r m_j = 0, \pm 1\) \((m_r, m_j\) are magnetic quantum numbers of \(A\)) in a free radiating atom \(A\). The dipole moment of quasi-molecular transition is assumed to vary very slowly versus \(r\) and cancelled during normalization of the profile. It will be assumed for all quasi-molecular potentials of interest \((\gamma = i, f)\), that the temperature \(T\) is sufficiently high, so, that the inequality takes place
\[
k_B T >> D_\varepsilon, \quad (16)
\]

where \(D_\varepsilon\) is the depth of the well of the potential \(U_b(r)\).

The construction of the profile is accomplished by splitting it in the two parts, one of which corresponds to the short-range interactions \(\Phi^{(1)}_i(\Delta\omega)\) and the other \(\Phi^{(2)}(\Delta\omega)\) to the long-range one \(\Phi^{(1)}_i(\Delta\omega) = \Phi^{(1)}_i(\Delta\omega) + \Phi^{(2)}(\Delta\omega)\). Accordingly the different types of trajectories correspond to the different ranges of the impact parameter variation in (12)-(15). For large enough \(b\) the trajectories are assumed to be rectilinear (the second type) and do not depend explicitly on the potential, but for small \(b\) it is necessary to introduce the physically reasonable effective “mean” potential \(U_b(r)\) like
\[
U_b(r) = A_i \exp(-\alpha_i r); \quad A_i = \sqrt{A_i A_f}, \quad \alpha_i = (\alpha_i + \alpha_f)/2. \quad (17)
\]

The trajectory of the first type in the potential \(U_b(r)\) then could be found analytically using the Takayanagi modified wave number approximation [8], while the characteristic value of the impact parameter \(R_b\), separating the two regions of its variation, could be found from the value of diffusion coefficient [9], obtained in the first order Chapman-Enskog approximation for the core part of potential, and equal to: \(R_b \approx \frac{1}{\alpha_0} \ln \left( \frac{A_i}{k_B T} \right)\).

The derivation of the asymptotic dependences of line profiles in the wings are accomplished on the basis of analysis of the behavior of \(G_{ij}(b,\varepsilon,\Delta\omega)\) on \(\Delta\omega\) as a function of the Massey parameter [1] \(\xi(\Delta\omega, b, \varepsilon) = |\Delta\omega \tau(b,\varepsilon)|\) \(\exp[\eta_{ij}(t,b,\varepsilon)]\). The Lorentz center of the profile corresponds to \(\Delta\omega\) small enough, where \(\xi(\Delta\omega, b, \varepsilon) < 1\). It is determined by the Van der Waals interaction, because the Weisskopf radius [4] \(b_w > R_b\), where \(b_w = (3\pi \left| C_{ij} - C_{ij} \right|) / (8\hbar < u >)^{1/5}\) according to (7). The wings correspond to large \(|\Delta\omega|\), where \(\xi(\Delta\omega, b, \varepsilon) > 1\), for the wide range of impact parameters and \(\varepsilon \sim k_B T\). If \(\xi(\Delta\omega, b, \varepsilon) > 1\), the stationary phase approximation could be applied to evaluate the integral, which value is determined in the vicinity of the stationary phase point \(t_{i}(\Delta\omega, b, \varepsilon)\), being the root of the equation \(\Delta\omega = 2\pi A_{ij}[R(t,b,\varepsilon)]h\). In fact there is superposition of contributions from different types of trajectories in the red and blue wings and both \(\Phi_i^{(1,2)}(\Delta\omega)\) have to be analyzed.
For certainty but without loss of generality consider the argument of cosine in (7) as negative. Then as the minimum of $\Delta U_{if}(r)$ practically always takes place at $r > R_0$ and hence $b > R_0$, the trajectories, which give the main contribution to $\Phi_{if}(\omega)$ at negative $\Delta \omega$ (*the red wing of the line*) are rectilinear as soon as $2\pi \Delta U_{if,\min}(r)/h > |\Delta \omega| > \langle u \rangle/b_w$, and this part of the red wing is described by the asymmetric classical statistical Van der Waals (V-W) distribution [4]

$$I_{\text{red}}(\omega) = \frac{2\pi n_x}{|\Delta \omega|^3/2} \exp\left(-\frac{4\pi^2}{9} \frac{|\Delta C_{6,\text{red}}|}{|\Delta \omega|} \right),$$

(18)

Remind that at $|\Delta \omega| < \langle u \rangle/b_w$, the profile has the symmetric Lorentz shape, and within UFCT for the scalar V-W interaction it gradually transforms around the corresponding Weisskopf frequency $\Omega_{\text{W}} = \langle u \rangle/b_w$ into the classical statistical V-W line shape that according to (17) for the red wing signifies the deceleration of its power decrease of intensity from the impact index 2 to the statistical index 3/2. At $\Delta \omega = \Delta U_{if,\min}/h$ the red satellite appears. For the negative $\Delta \omega < 2\pi \Delta U_{if,\min}(r)/h$ no real roots exist for equation $\Delta \omega = 2\pi \Delta U_{if}(R(t,b,e))/h$, and $\Phi_{if}(\Delta \omega)$ decrease exponentially $\sim \exp[-\xi(\Delta \omega,b,e)]$ with increasing $|\Delta \omega|$. It is to be noted that this part of the red wing is determined by the contribution of the second type of trajectories. Thus the line profile should exhibit the strong exponential decrease in the red wing at detunings $\Delta \omega < \Delta \omega_{\text{red}} = 2\pi \Delta U_{if,\min,\text{eff}}/h$, where $\Delta U_{\text{min,\text{eff}}}$ is some average minimum value of the potential differences of initial and final states. The value of $\Delta \omega_{\text{red}}$ is specific for the each A-X pair and could be estimated from the approximate potential curves, including attractive and repulsive parts. For the systems of interest $\Delta \omega_{\text{red}}$ may vary in the wide range from hundreds to thousands of cm$^{-1}$.

For the positive $\Delta \omega$ (*the blue wing of the line*) the situation is different. At $|\Delta \omega| < \langle u \rangle/b_w$ the blue wing has the Lorentz part symmetric with respect to the red wing, and within UFCT for the second type of trajectories. But it gradually vanishes around the corresponding Weisskopf frequency $\Omega_{\text{W}} = \langle u \rangle/b_w$, according to [4], if $\Delta C_{6,\text{eff}} < 0$. Depending on the specific interaction potentials the range of positive $\Delta \omega$ for which equation $\Delta \omega = 2\pi \Delta U_{if}(R(t,b,e))/h$ has real solution may be practically unrestricted or restricted from above. If the maximum of $\Delta U_{if}(r)$ exists then for $\Delta \omega > 2\pi \Delta U_{\text{if,\max}}/h$ the roots are complex, and corresponding $G_{if}(b,e,\Delta \omega)$ decreases exponentially $\sim \exp[-\xi(\Delta \omega,b,e)]$ with increasing $\Delta \omega$. Since the interaction $\Delta U_{if}(r)$ usually takes positive values at $r < R_0$, which correspond to dominance of the repulsive core, the Massey parameter is of the order of $\Delta \omega/\alpha_0\langle u \rangle$. If $\Delta U_{if}(r)$ have maximum, the blue satellite will appear at $\Delta \omega = \Delta U_{\text{if,\max}}$. It is to be noted that this satellite is usually very far from the center of the line (up to several thousands of cm$^{-1}$). With increasing $\Delta \omega$ the equation $2\pi \Delta U_{\text{if,\max}}/h = \Delta \omega$ will have real roots for increasing energy $e$, that will lead to exponential decrease of $\Phi_{if}^{(1)}(\Delta \omega)$ with increasing $\Delta \omega$ due to thermal average in (13). Therefore the strong exponential decrease of the blue wing should occur at detunings $\Delta \omega < \Delta \omega_{\text{blue}} = \alpha_0\langle u \rangle$ that effectively is shown up as its cutting. Typically $\alpha_0$ is about 2-3 Å$^{-1}$.

Thus the described procedure allows to obtain the total profile with its smooth transition from the impact to the quasistatic region of the detuning from line center $\Delta \omega$ and to take properly into account the characteristic repulsive core of the interaction potential that leads to the exponentially decreasing of its far wings.

The difficulties of performing explicitly such kind of calculations and especially lacking of the accurate independent information about diatomic potential curves pushed earlier to search for more simple procedures of calculations that also would contain the impact and quasistatic contributions in the total line profile. And indeed, Stormberg [10] proposed to construct the approximate total profiles on the basis of convolution of the purely impact and purely quasistatic contours due to Van der Waals broadening [4] that allowed to arrive to closed analytical expression in terms of the Faddeev function [10]. This approximate method became very popular in the applied spectroscopy, although it gives
wrong behaviour of the far profile wings due to the appearance there the impact contribution. It was recognized that using such kind of profiles leads to the dramatic overestimation of the radiation transfer in the wings, and the various empirical procedures of far profile wings artificial cutting were proposed, that alas had no theoretical justification background. Now the presented above study allows to provide physically justified simple receipts of wing cutting procedure, that would improve the wings behaviour of convolved total profile [10]. Indeed, as follows from the above consideration the total profile [10] could be corrected in the following way:

\[
\text{convII} \mathcal{Z} \mathcal{Z}, \quad \text{where} \quad c_{f}\left(\mathcal{Z}\right) = \begin{cases} 
1, & \text{if } \Delta \omega < 0, \Delta \omega^{(\text{red})} > |\Delta \omega| > 0, \\
\exp\left[-\kappa_{f}\left(|\Delta \omega| - \Delta \omega^{(\text{red})}\right)\right], & \text{if } \Delta \omega < 0, |\Delta \omega| > \Delta \omega^{(\text{red})} > 0,
\end{cases}
\]

(19)

\[
\Delta \omega^{(\text{red})}_{c,f} = \frac{\Delta U_{Uf,\text{min}}}{h}, \quad \text{and} \quad \kappa_{f} = \left(\frac{1}{6} \frac{\kappa_{h} T}{\mu} \left| \frac{d^2 U_{Uf}(R)}{d R^2} \right|_{R=R_{\text{min}}} \right)^{-1/3}.
\]

(20)

Here \(\Delta U_{Uf,\text{min}}=U_{f}(R)-U_{f}(R)\) is the minimum of the difference of potentials at \(R=R_{\text{min}}\). And in the blue wing the partial cutting function \(c_{b}(\Delta \omega)\) could be presented in the form:

\[
\mathcal{Z}_{\omega} \mathcal{Z}_{\mathcal{Z}}:=\begin{cases} 
1, & \text{if } \Omega_{w,b} > \Delta \omega > 0, \\
0, & \text{if } \Delta \omega > \Omega_{w,b} > 0,
\end{cases}
\]

(21)

where the Weisskopf \(\Omega_{w,b}\) frequency is marked also by the labels of the upper and lower levels of radiative transition. Thus the receipts (19)-(21) correct the behavior of the approximate total profile [10].

Resuming it could be stated: * for the binary case the impact limit of Van der Waals broadening was found exactly taking into account the degeneracy of quasimolecular states; ** the general asymptotic dependences of the red and blue wings of the profile were established on the basis of parameterized with the help of ab initio calculations Buckingham potential and UFCT methods; *** the receipts of cutting procedure for improving the line wings behaviour of the approximate total profiles, obtained by convolution of the Van der Waals pure impact and pure statistical profiles are formulated.

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