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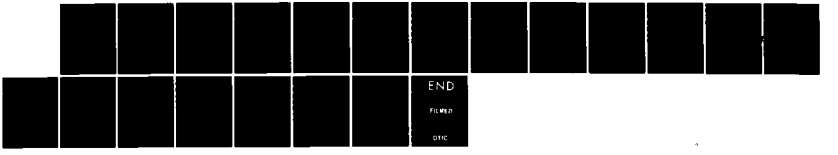

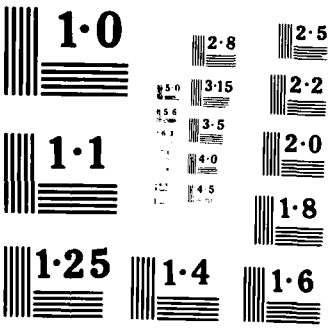
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Average Collisional Vibrational Energy Transfer Quantities and the Inversion Temperature

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Energy Transfer	Tin
High Temperature	Unimolecular Reaction
Inversion Temperature	Vibrational Relaxation

20 ABSTRACT (Continue on reverse side if necessary and identify by block number)

Collisional efficiencies for vibrational energy transfer have previously been related to the quantities $\langle \Delta E \rangle_d$ and $\langle \Delta E \rangle_{all}$. These quantities have been examined here as a function of molecular complexity, critical reaction threshold, E_o, temperature and energy transfer step size. Model calculations were made for the decomposition of nitryl chloride and for the isomerizations of methyl isocyanide, cyclopropane and cycloheptatriene. For large step size and low temperature, $\langle \Delta E \rangle_{all} \rightarrow \langle \Delta E \rangle_d$ at

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Abstract (Continued)

high temperatures up transitions dominate and $\langle \Delta E \rangle_{all} = \langle \Delta E \rangle_{d}$. An inversion temperature T_I is predicted when $p_{up} = p_{down}$; this temperature is quasi independent of step size and dependent on molecular energy and molecular complexity. T_I is used to compute an effective temperature which can be used to give an analytical expression which relates $\langle \Delta E \rangle_{all}$ and $\langle \Delta E \rangle_{d}$.

AVERAGE COLLISIONAL VIBRATIONAL ENERGY TRANSFER QUANTITIES AND THE INVERSION TEMPERATURE

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Abstract

Collisional efficiencies for vibrational energy transfer have previously been related to the quantities, $\langle\Delta E\rangle_d$ and $\langle\Delta E\rangle_{all}$. These quantities have been examined here as a function of molecular complexity, critical reaction threshold, E_o, temperature and energy transfer step size. Model calculations were made for the decomposition of nitryl chloride and for the isomerizations of methyl isocyanide, cyclopropane and cycloheptatriene. For large step size and low temperature, $\langle\Delta E\rangle_{all} = -\langle\Delta E\rangle_d$; at high temperatures up transitions dominate and $\langle\Delta E\rangle_{all} = \langle\Delta E\rangle_d$. An inversion temperature T_I is predicted when $p_{up} = p_{down}$; this temperature is quasi-independent of step size and dependent on molecular energy and molecular complexity. T_I is used to compute an effective temperature which can be used to give an analytical expression which relates $\langle\Delta E\rangle_{all}$ and $\langle\Delta E\rangle_d$

Introduction

The collisional vibrational deactivation efficiency, β_c, has been used successfully to parameterize thermal unimolecular reactions involving weak colliders. Tardy and Rabinovitch[1,2] and Troe[3] have developed expressions relating β_c to average energy transferred quantities, $\langle\Delta E\rangle_d$ and $\langle\Delta E\rangle_{all}$, respectively. These quantities are defined as:

$$\langle\Delta E\rangle_d = \int_o^E (E'-E)P(E',E)dE' \Big/ \int_o^E P(E',E)dE'$$

$$\langle\Delta E\rangle_{all} = \int_o^\infty (E'-E)P(E',E)dE' \Big/ \int_o^\infty P(E',E)dE'$$

also,

$$\langle\Delta E\rangle_u = \int_E^\infty (E'-E)P(E',E)dE' \Big/ \int_E^\infty P(E',E)dE'$$

where $P(E',E)$ is the probability that a molecule with internal energy E will have E' after collision; additionally,

$$\langle\Delta E\rangle_{all} = \langle p\rangle_{up}\,\langle\Delta E\rangle_u - \langle p\rangle_{down}\,\langle\Delta E\rangle_d \quad ;$$

where,

$$\langle p\rangle_{up} = \int_E^\infty P(E',E)dE' \Big/ \int_o^\infty P(E',E)dE'$$

and

$$\langle p\rangle_{down} = \int_o^E P(E',E)dE' \Big/ \int_o^\infty P(E',E)dE'$$

These quantities are related by completeness, $\int_o^\infty P(E',E)dE'=1$, and detailed balance, $(P(E',E)/P(E,E')=\rho_{E'}/\rho_E \exp[-(E'-E)/RT])$. Note that the sign convention makes $\langle\Delta E\rangle_{all} = -\langle\Delta E\rangle_d$ when $\langle p\rangle_{down} = 1$, and $\langle\Delta E\rangle_{all} = \langle\Delta E\rangle_u$ when $\langle p\rangle_{down} = 0$. Although the $P(E',E)$ are not known *a priori*, various limiting model types have been used for comparative purposes (step ladder, Gaussian, exponential, etc).[1]

Some confusion[2] has resulted because $\langle\Delta E\rangle_d$ and $\langle\Delta E\rangle_{all}$ have both been used in the literature[4-7]. Recently, Gilbert[4] has shown that $\langle\Delta E\rangle_d$ is the more appropriate quantity to use in parameterizing β_c. Oref and coworkers in a series of papers[5] have given exhaustive treatments of these parameters and their interrelations, for the case especially of Boltzmann-like transition

probabilities. For a given $P(E',E)$ model, Barker[6] has also shown that $\langle\Delta E\rangle_{all}$ can change sign with temperature even though $\langle\Delta E\rangle_d$ does not.

In the present work, we illustrate dependence of the ratio, $\gamma=\langle\Delta E\rangle_{all}/\langle\Delta E\rangle_d$, on the quantities $\langle\Delta E_d\rangle$ and temperature and on reactant properties i.e. internal molecular parameters and critical energy for reaction, E_o.

Calculations

Four prototype model reactions were used: decomposition of nitryl chloride and the isomerizations of methyl isocyanide, cyclopropane and cycloheptatriene. These reactants reflect differences in vibrational frequency patterns and molecular complexity, excitation levels and temperatures. Table 1 exhibits some pertinent quantities.

For simplicity of exposition, a step ladder model of the collisional transition probabilities with step size ΔE was used ($\Delta E = \langle\Delta E\rangle_u = \langle\Delta E\rangle_d$), and the probabilities were computed at $E=E_o$:

$$p_{up}/p_{down} = P(E_o+\Delta E,E_o)/P(E_o,E_o+\Delta E) = (\rho_{E_o+\Delta E}/\rho_{E_o})\exp(-\Delta E/RT)$$

It is seen that the general definition of the energy ratio, $\gamma=\langle\Delta E\rangle_{all}/\langle\Delta E\rangle_d$, takes the form of eq. 1 for a step ladder model and is a function of step size, temperature, excitation level (critical reaction threshold) and molecular complexity; the last two dependencies enter through the density of states:

$$\gamma_{SL} = (p_{up}-p_{down}) = -[1 - p_{up}/p_{down}]/[1 + p_{up}/p_{down}]$$

$$= -(1-(\rho_{E_o+\Delta E}/\rho_{E_o})\exp(-\Delta E/RT))/(1+(\rho_{E_o+\Delta E}/\rho_{E_o})\exp(-\Delta E/RT)) \qquad (1)$$

A plot of γ_{SL} vs $(\rho_{E_o+\Delta E}/\rho_{E_o})\exp(-\Delta E/RT)$ for a range of temperatures (200-16000 K) and step sizes (100-3200 cm^{-1}) is shown in Fig. 1 for the prototype systems. As required, a universal plot is observed.

Equation (1) is simplified by replacing the density of states for the molecule by the density for s classical oscillators. Define $p_r=(p_{up}/p_{down})_{cl}$ as

$$p_r = \left[1 + \frac{\Delta E}{E_o}\right]^{s-1} \exp[-\Delta E/RT] > 0;$$

so, $$\gamma_{SL} = -(1-p_r)/(1+p_r).$$

For the case $\Delta E/E_o << 1$,

$$p_r = \left(1+\frac{\Delta E}{E_o}\right)^{s-1} e^{-\Delta E/RT} \simeq [1+(s-1)\Delta E/E_o]e^{-\Delta E/RT} \quad . \qquad (2)$$

Thus, $$\gamma_{SL} < 0 \text{ for } p_r > 1; \text{ or } \gamma_{SL} > 0 \text{ for } p_r < 1.$$

These limits can be attained at high and low temperatures, respectively. In the low temperature limit, the Boltzmann factor dominates so that γ_{SL} is a function mainly of ΔE and T. In this limit, γ_{SL} increases from -1 with decrease in ΔE and with increase in temperature. In the high temperature limit, i.e. $\exp(-\Delta E/RT)\sim 1$, the density ratio dominates and γ_{SL} is a function of ΔE and $(s-1)/E_o$; γ_{SL} decreases from unity with decrease in ΔE.

At the inversion temperature, T_I, the Boltzmann and density factors compensate one another, so that $p_{up}=p_{down}$ and $p_r=1$. T_I is sufficiently greater than typical reaction temperatures so that it is only approached for reactants having an unusually small E_o and/or a large value of s. For the experimental systems under examination, this temperature might only be realized for cycloheptatriene (Table 1). T_I is the temperature for which E_o is coincident with the maximum in the classical energy distribution. It is evident from eq. (2) that $T_I=E_o/[(s-1)R]$. Thus, to this approximation, T_I is independent of step size (ΔE). Indeed for the prototype systems, only a weak dependence on ΔE is exhibited in Table 1. Also to be noted from Table 1 is that a larger reactant having a high E_o shows similar values (i.e. density ratios and T_I) to a smaller reactant having a low E_o, eg. C_3H_6 and CH_3NC .

When $\rho_{E_o+\Delta E}/\rho_{E_o}$ is only a weak function of molecular complexity, i.e. for $(s-1)\Delta E << E_o$, (see Table 1 for the case, $\Delta E < 400\ cm^{-1}$), γ_{SL} is expected to be a universal function of $\Delta E/RT$. To take the general effect of molecular complexity

into account, an effective temperature can be used. Tardy and Rabinovitch[1] have done this by using a dimensionless parameter, $\langle\Delta E\rangle/\langle E^{+}\rangle$, where,

$$\langle E^{+}\rangle = \int_{E_o}^{\infty} (E-E_o)\rho(E)\ e^{-E/RT}dE \Big/ \int_{E_o}^{\infty} \rho(E)\ e^{-E/RT}\ dE$$

We now define an effective temperature, T_e as the temperature at which $p_r=\exp(-\Delta E/RT_e)$; so that $T_e = T/(1-(s-1)RT/E_o) = T/(1-T/T_I) = T\ T_I/(T_I-T)$; s is calculated from the density of states ratio at E_o i.e. $s=1+\ln(\rho_{E_o+\Delta E}/\rho_{E_o})/\ln((E_o+\Delta E)/RT)$. For $T<<T_I$, $T_e \longrightarrow T$, and for $T>>T_I$, $T_e \longrightarrow -T_I$. A discontinuity occurs when $T = T_I$; in this case $1/T_e = 0$. Figure 2 illustrates the dependence of γ_{SL} on T_e for the prototype systems: a near-universal curve results. A shotgun pattern results if $\langle\Delta E\rangle/RT$ is used (not shown).

Earlier work in the literature for an exponential model[3] related $\langle\Delta E\rangle_d$ and $\langle\Delta E\rangle_{all}$ by the equation, $\gamma_{Exp} = \dfrac{\langle\Delta E\rangle_{all}}{\langle\Delta E\rangle_d} = \dfrac{-\langle\Delta E\rangle_d}{\langle\Delta E\rangle_d+RT} = \dfrac{-\langle\Delta E\rangle_d}{\langle\Delta E\rangle_d+F_E RT}$ (3)

The F_E correction was added in later work[8] and was stated to be near unity, in practice. As has been noted[6], this expression does not take into account the required sign change for γ_{Exp}. In the weak collision limit (β_c <0.03) or $\langle\Delta E\rangle_d<<kT$), $\gamma_{Exp} \simeq -\langle\Delta E\rangle_d/F_E kT$, i.e. γ_{Exp} is linear with $\langle\Delta E\rangle_d$. For the region ($|\gamma_{SL}|<0.4$), the present work illustrates that γ_{SL} is linear with $\langle\Delta E\rangle_d$ with a slope of $\sim -1/(2RT_e)$ (Fig 2); the slope depends on T_e, which is usually positive. Additionally, if eq (3) is adopted for the step ladder case, *then it is seen that* $F_E = 2[1+(s-1)RT/E_o]$ *or* $F_E>2$, *always*.

Using T_e, eq 1 gives $\gamma_{SL}=-\tanh(\Delta E/2RT_e)$. Thus we have determined a relation which is valid for all step sizes and all temperatures and which is substantially easier to use than solving an integro-differential equation[4]. From the above relation, $\langle\Delta E\rangle_{all}$ is easily computed from $\langle\Delta E\rangle_d$ and T_e. Due to the transcendental nature of the function, indirect methods are required

to obtain $\langle\Delta E\rangle_d$ from $\langle\Delta E\rangle_{all}$ and T_e (Regula Falsi, Newton-Raphson or, simply, by iteration on Fig 2).

In future work, we will present the results for the exponential model which can be directly compared to the expression developed by Troe[8]; different analytical expressions for ρ_E will also be evaluated.

Conclusions

These calculations demonstrate that for low temperature and large step size (p_{down}~1), $\langle\Delta E\rangle_{all} = -\langle\Delta E\rangle_d$; as step size decreases, or temperature increases, $\langle\Delta E\rangle_{all}$ increases. An inversion temperature T_I is reached when $p_{down}=p_{up}$; for this condition $\langle\Delta E\rangle_{all}=0$. With increasing temperature, $p_{up} > p_{down}$, and $\langle\Delta E\rangle_{all}$ becomes positive; in the limit $\langle\Delta E\rangle_{all}=\langle\Delta E\rangle_d$. In general, T_I is much larger than normal reaction temperatures; T_I decreases with molecular complexity and increases with E_o. Thus, for large molecules with low E_o, the difference between $-\langle\Delta E\rangle_{all}$ and $\langle\Delta E\rangle_d$ will be large.

The functional dependence of the density of states on excitation level and number of oscillators has been used to show that a large molecule with a high E_o behaves in a manner similar to a small molecule with low E_o; and to develop a universal equation relating γ_{SL} to $\langle\Delta E\rangle_d$ and T_e.

Acknowledgment

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Table 1 Reactant Parameters and Calculational Results

Reactant	No Vibs	E_o (cm^{-1})	T_r[a] (K)	Class s at E_o	$\rho E_o + \Delta E / \rho E_o$ ΔE (cm^{-1})					Approx[b] T_I	Exact T_I[c] ΔE(cm^{-1})				
					100	200	400	800	1600		100	200	400	800	1600
NO_2Cl	6	10325	455	5 1	1 040	1 081	1 167	1 355	1 803	3697	3690	3704	3733	3791	3903
CH_3NC	12	13300	546	7 9	1 053	1 118	1 226	1 498	2 210	2813	2799	2806	2820	2847	2902
$C-C_3H_6$	21	21875	720	13 2	1 057	1 118	1 248	1 554	2 389	2634	2585	2589	2597	2613	2644
$C-C_4H_8$	39	18000	650	20 0	1 111	1 233	1 518	2 292	5 42	1380	1372	1374	1378	1388	1406

a) T_r is the thermal reaction temperature

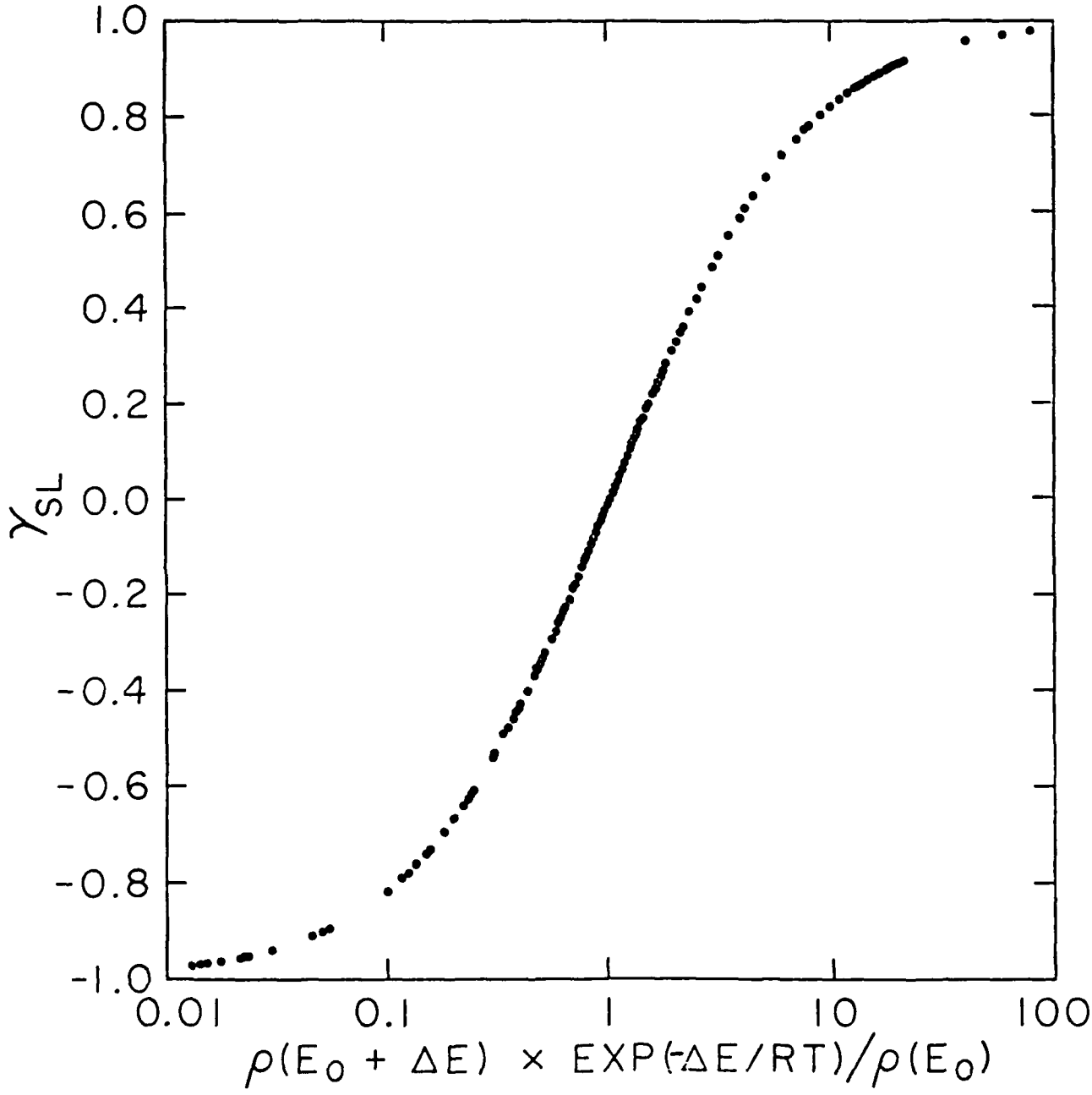
b) T_I is calculated from the $E_o/(s-1)R$ approximation in text

c) T_I is the exact temperature such that $p_{up} = p_{down}$ for given step size of ΔE

FIGURE CAPTIONS

1. Plot of γ_{SL} vs $(\rho_{E_o+\Delta E} / \rho_{E_o})\ e^{(-\Delta E/RT)}$ for nitryl chloride, methyl isocyanide, cyclopropane and cycloheptatriene for step sizes of 100, 200, 400, 800, 1600 and 3200 cm^{-1}, each at 250, 500, 1000, 2000, 4000 and 8000 K.

2. Plot of γ_{SL} vs $\langle \Delta E \rangle_d / RT_e$; see legend of Figure 1. T_e calculated from expression given in text.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0.8
0.6
0.4
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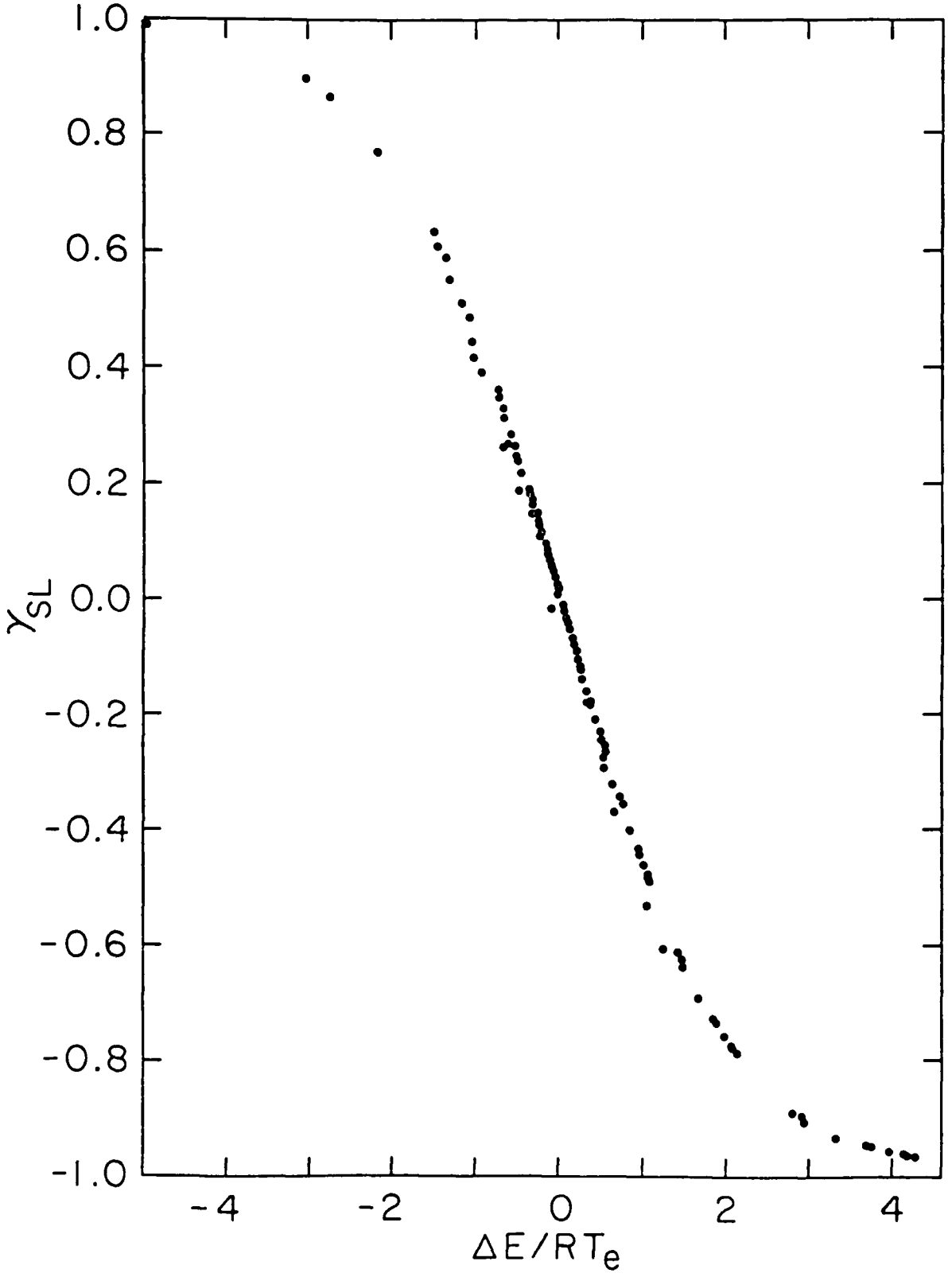
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
γ_{SL}
0.01
0.1
1
10
100
$\rho(E_0 + \Delta E) \times EXP(-\Delta E/RT)/\rho(E_0)$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-0.4
-0.6
-0.8
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γ_{SL}
-4
-2
0
2
4
$\Delta E/RT_e$

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