

TESTING THE APPLICABILITY OF SCALING LAW FOR COLLISIONAL RATE COEFFICIENTS

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Calculation of collisional rate coefficients is a challenging and difficult task. When these data are not available, their values may be estimated using a scaling law. In some investigations, we have utilized a scaling law. Accurate collisional rate coefficients for cyclopropenylidene ($c\text{-C}_3\text{H}_2$) as a complete set are available, and thus it may be appropriate occasion to test the applicability of that scaling law. We have considered 50 rotational levels of each of the ortho and para species of $c\text{-C}_3\text{H}_2$ having energies up to 91.53 cm^{-1} and 87.21 cm^{-1} , respectively. We have compared the results of radiative transfer using accurate collisional rate coefficients with those obtained using the scaling law, and have found that the results of the scaling law are qualitative. Hence, for getting the qualitative behaviour of an analysis, the use of the scaling law is quite reasonable.

Keywords: *ISM molecules: saling law: Sobolev LVG analysis: radiative transfer*

1. Introduction. Calculation of collisional rate coefficients is a challenging and difficult task [1], and therefore, such data are available for a limited number of molecules. As these data were not available, we [2-4] have used a scaling law

$$C(J'_{k'_a, k'_c} \rightarrow J_{k_a, k_c}) = \frac{1 \cdot 10^{-11}}{2J'+1} \sqrt{T} \quad (1)$$

for estimation of collisional rate coefficients in the downward direction $J'_{k'_a, k'_c} \rightarrow J_{k_a, k_c}$. This is cross section times the relative velocity between the target and the colliding partner. A cross section σ may be taken as πa_0^2 , where $a_0 = 0.52917\text{ \AA}$ is the Bohr radius. Hence, $\sigma \approx 10^{-16}\text{ cm}^2$. For a velocity $v \approx 1\text{ m/s}$, we have $\langle \sigma v \rangle \approx 10^{-11}\text{ cm}^3/\text{s}$. Collisional rate coefficients for excitation (upward direction) may be calculated using the detailed equilibrium:

$$C(J_{K_a, K_c} \rightarrow J'_{K'_a, K'_c}) = \left[\frac{2J'+1}{2J+1} \right] \exp \left[-\frac{\Delta E}{kT} \right] C(J'_{K'_a, K'_c} \rightarrow J_{K_a, K_c}), \quad (2)$$

where, ΔE is the energy difference between the levels J_{k_a, k_c} and $J'_{k'_a, k'_c}$.

Khalifa et al. [5] have calculated accurate collisional rate coefficients for rotational transitions in the ground vibrational state of cyclopropenylidene ($c\text{-C}_3\text{H}_2$) due to collisions with the He atom. It has been a regular practice to replace H_2 molecule (which is the most abundant molecule in a molecular region) by He atom [6-9], as both of them have two protons and two electrons. It is because

the calculations with He atom are easier as compared to those with H_2 molecule.

The cyclopropenylidene ($c\text{-}C_3H_2$) is a planar asymmetric top molecule having C_{2v} symmetry and large electric dipole moment $\mu = 3.27$ Debye [10] lying along the b -axis of inertia. Earlier, the electric dipole moment μ was calculated as 3.32 Debye [11]. The cyclopropenylidene has been analyzed in the terrestrial laboratories from time to time [12,13]. After H_2CO [14], the $c\text{-}C_3H_2$ is the second molecule to show the phenomenon of anomalous absorption. Following first detection of $c\text{-}C_3H_2$ by Matthews et al. [15], Madden et al. [16] found $c\text{-}C_3H_2$ ubiquitous, through its transition $2_{20}\text{-}2_{11}$ at 21.587 GHz, which was found in anomalous

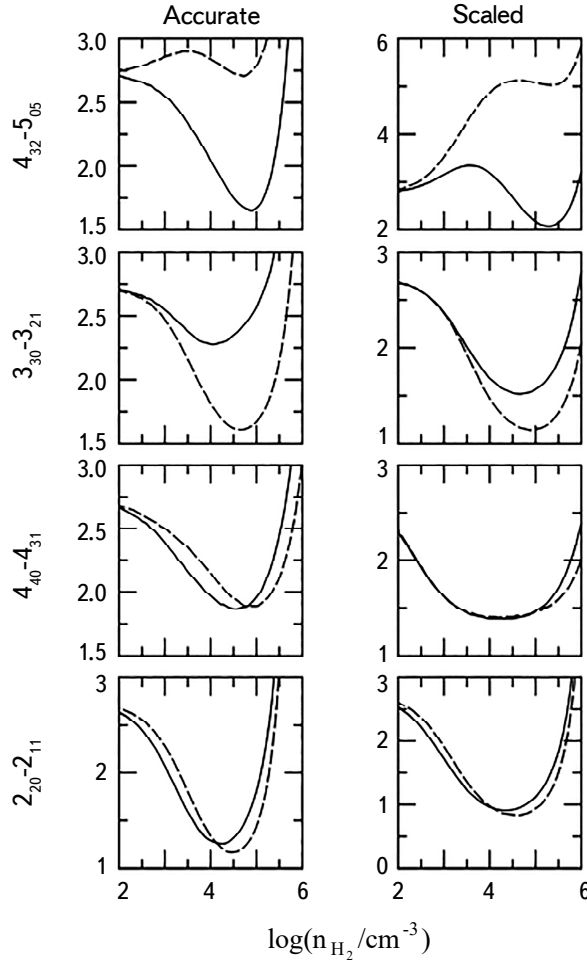


Fig.1. Variation of excitation temperatures T_{ex} (K) versus molecular hydrogen density n_{H_2} for the accurate and scaled collisional rate coefficients, written at the top, at kinetic temperature 30 K, for anomalous absorption lines of cyclopropenylidene, written on the left. Solid line is for $\gamma = 10^{-5} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$, and the dotted line for $\gamma = 10^{-6} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$.

absorption (the absorption against the cosmic microwave background having the background temperature of 2.73 K). Cox et al. [17], however, reported this line in emission in the planetary nebula NGC 7027. Because of two equivalent hydrogen atoms, the c -C₃H₂ has ortho and para species. For each species, the collisional rate coefficients are available for 50 rotational levels having energies up to 91.53 cm⁻¹ and 87.21 cm⁻¹, respectively. Using these accurate collisional rate coefficients, Sharma and Chandra [18] have performed Sobolev analysis of both species and have discussed results for four, $2_{2,0}$ - $2_{1,1}$, $4_{4,0}$ - $4_{3,1}$, $3_{3,0}$ - $3_{2,1}$ and $4_{3,2}$ - $5_{0,5}$, transitions showing anomalous absorption, and two transitions, $4_{0,4}$ - $3_{3,1}$, $5_{1,4}$ - $4_{4,1}$, showing the weak MASER action. One transition $1_{1,0}$ - $1_{0,1}$ connection the ground state of ortho species was also considered.

In order to test the applicability of the scaling law (1), we have repeated the simulation of Sharma and Chandra [18] where the accurate collisional rate coefficients have been replaced by the values obtained using the scaling law (1). The two sets of results are compared and the conclusions are drawn. The parameter

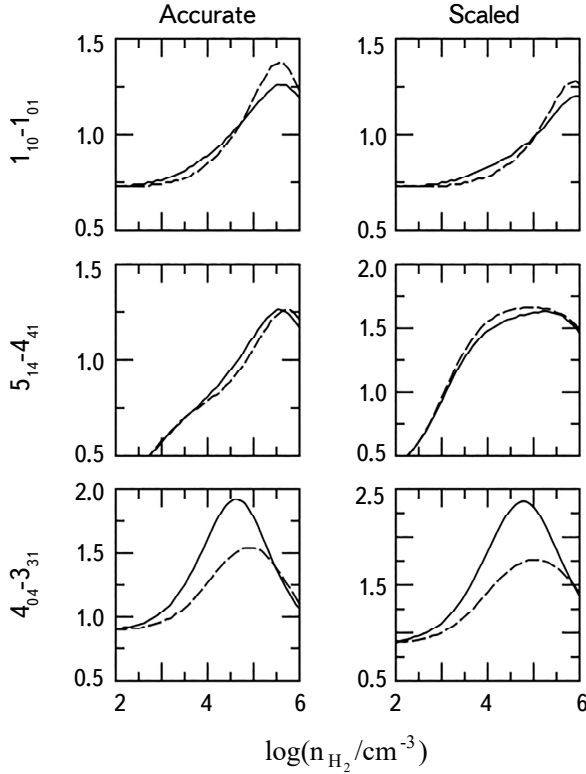


Fig. 2 Variation of $n_e g_u / n_l g_l$ versus molecular hydrogen density n_{H_2} for the accurate and scaled collisional rate coefficients, written at the top, at kinetic temperature 30 K, for the transitions of cyclopropenylidene, written on the left. Solid line is for $\gamma = 10^{-5} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$, and the dotted line for $\gamma = 10^{-6} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$.

γ is defined as $\gamma = n_{mol}/(dv_r/dr)$, where n_{mol} denotes the density of the species of molecule, and dv_r/dr is the velocity-gradient in the region.

2. Results and discussion. Details of calculations and information about the data used are available in Sharma and Chandra [18]. To check the applicability of equation (1), we have repeated the simulation of Sharma and Chandra [18] as such, where the accurate collisional rate coefficients of Khalifa et al. [5] are replaced by those obtained by using equation (1). Comparison of results for kinetic temperature of 30 K is shown in Fig.1 for four anomalous absorption lines and in Fig.2 for two weak MASER lines and the line connecting the ground state of ortho species. The Figures show that though the results may vary significantly, but their qualitative behaviour remains the same. Similar results have been obtained for other kinetic temperatures, 10, 20, 40, 50 K also. The results support the idea that when accurate collisional rate coefficients are not available, the scaling law expressed by equation (1) may be used to get qualitative behaviour of results of investigation.

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ПРОВЕРКА ПРИМЕНИМОСТИ ЗАКОНА ПОДОБИЯ ДЛЯ СТОЛКНОВИТЕЛЬНЫХ КОЭФФИЦИЕНТОВ

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Вычисление столкновительных коэффициентов является сложной и трудной задачей. Когда эти данные недоступны, их значения могут быть оценены с использованием закона скейлинга (закон подобия/масштабная инвариантность).

В некоторых исследованиях мы использовали закон подобия. Точные коэффициенты скорости столкновений для циклопропенилидена ($c\text{-C}_3\text{H}_2$) доступны в виде полного набора, что позволило анализировать возможность применения закона подобия. Рассмотрено по 50 вращательных уровней каждого из орто- и пара-видов $c\text{-C}_3\text{H}_2$ с энергиями до 91.53 см^{-1} и 87.21 см^{-1} , соответственно. Сравнение результатов переноса излучения с использованием точных столкновительных коэффициентов с результатами, полученными с использованием закона подобия, показало, что результаты закона подобия являются качественными. Следовательно, для получения качественного поведения анализа использование закона подобия вполне разумно.

Ключевые слова: молекулы: закон подобия: LVG анализ Соболева: перенос излучения

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