Detection of rotational lines of NaSH molecule

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Laboratory detection of NaSH molecule in absorption has been reported by Kagi and Kawaguchi, *Astrophys J*, **491** (1997) L129. They observed only *a*-type rotational transitions of the molecule. The reason for not observing *b*-type rotational transitions was assigned to a small value of *b*-component of electric dipole moment (μ_b=0.63 D) as compared to *a*-component of electric dipole moment (μ_a=8.91 D) of the molecule. The *b*-type transitions may be detected in emission in interstellar medium having low densities. However, it is not feasible to detect *b*-type rotational transitions in the absorption spectrum.

By using a source-modulated millimeter/sub-millimeter spectrometer, Kagi and Kawaguchi[1] recorded the absorption rotational spectrum of sodium hydrosulphide, NaSH, molecule in the laboratory. The molecule NaSH was generated by a dc discharge in a mixture of Na vapour, H_2S, and Ar by making use of high temperature cell. The NaSH is an asymmetric top molecule and its electric dipole moment can be resolved into two components: μ_a = 8.91 D and μ_b = 0.63 D along the *a*- and *b*-axes of inertia, respectively. Hence, the molecule is supposed to generate both *a*- and *b*-type rotational lines. Kagi and Kawaguchi[1] recorded *a*-type transitions with great accuracy, but could not succeed in recording the *b*-type transitions. The reason for not observing *b*-type transitions has been assigned to a small value of μ_b as compared to that of μ_a. We find that *b*-type transitions may be detected in emission in interstellar medium having low densities. However, the detection of *b*-type transitions in the absorption would not be feasible.

Einstein A-coefficients - In order to understand about probabilities of radiative transitions in the NaSH molecule, let us first calculate Einstein A-coefficients for *a*- and *b*-type rotational transitions in the ground vibrational state of the molecule. The

details of the calculation of Einstein A-coefficients for *a*-type rotational transitions in an asymmetric top molecule have been discussed by Chandra and Sahu[2], Chandra and Sharma[3] and Chandra and Rashmi[4]. These transitions are governed by the selection rules:

$$\begin{aligned} J: &\quad \triangle J = 0, \pm 1 \\ K_a, K_c: &\quad \text{odd, even} \longleftrightarrow \text{odd, odd} \\ &\quad \text{even, even} \longleftrightarrow \text{even, odd} \end{aligned}$$

By using the molecular constants, and distortional constants derived by Kagi and Kawaguchi[1], the values of the Einstein A-coefficients for *a*-type rotational transitions in the ground vibrational state of NaSH between the levels up to 20 cm^{-1} are computed and are given in Tab. 1.

The details of the calculation of Einstein A-coefficients for *b*-type rotational transitions in an asymmetric top molecule have been discussed by Chandra *et al.*, and Sharma and Chandra[5−7]. These transitions are governed by the selection rules:

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Computed values of the Einstein A-coefficients for *b*-type rotational transitions in the ground vibrational state of NaSH between the levels up to 20 cm^{-1} are given in Tab. 2.

Discussion - The A-coefficients for *b*-type transitions are of the same order of magnitude as those for *a*-type transitions. However, it happens owing to large frequencies for *b*-type transitions as compared to those for *a*-type transitions. It is further interesting to notice from the energy level diagram of the molecule that, for *a*-type transitions, the energy levels can be grouped into two parts: (i) the levels with low energies, namely, $0_{0,0}$, $1_{0,1}$, $2_{0,2}$, $3_{0,3}$, $4_{0,4}$, $5_{0,5}$, & $6_{0,6}$, and (ii) the levels with high energies, namely, $1_{1,1}$, $1_{1,0}$, $2_{1,2}$, $2_{1,1}$, $7_{0,7}$, $3_{1,3}$, $3_{1,2}$ and so on. The $7_{0,7} \rightarrow 6_{0,6}$ is the only *a*-type transition which connects these two groups (i) and (ii) of the energy levels. It shows that *a*-type transitions between the energy levels of group (ii) (except those between the backbone levels $7_{0,7}$, $8_{0,8}$, $9_{0,9}$ etc.) will cascade down to the level $1_{1,1}$. From this level $1_{1,1}$ there is no *a*-type transition in the downward direction. Thus, the level $1_{1,1}$ is essentially a metastable one, and from this level,

the molecule can de-excite either through the b-type transitions $1_{1,1} \rightarrow 0_{0,0}$, and $1_{1,1} \rightarrow 2_{0,2}$ at 298.7 and 262.8 GHz, respectively, or owing to the collisions with H_2 molecules of H atoms. Therefore, when the density (pressure) in the region is low, the possibility of collisional de-excitation would be very small and the aforesaid b-type emission transitions may be observed. Further, since the A-coefficient for the a-type transition $1_{1,0} \rightarrow 1_{1,1}$ is 1.19 x 10^{-12} s^{-1}, the possibility of detection of the b-type transition $1_{1,0} \rightarrow 1_{0,1}$ at 286.9 GHz (A-coefficient = 5.45 x 10^{-5} s^{-1}) in emission spectrum cannot be ruled out. Thus, there is a reasonably good possibility of the detection of b-type transitions $1_{1,1} \rightarrow 0_{0,0}$, $1_{1,1} \rightarrow 2_{0,2}$, and $1_{1,0} \rightarrow 1_{0,1}$ at 298.7, 262.8, and 286.9 GHz, respectively, in emission spectrum of an interstellar medium having low density. The energy level diagram and A-coefficients show that the detection of b-type transitions in absorption would not be feasible, because in a transition from a lower energy level to an upper energy level, the probability for an a-type transition is very large in comparison to that for a b-type transition.

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Table 1 - Einstein A-coefficients for *a*-type transitions

Transition	A-coefficient (s^{-1})	Transition	A-coefficient (s^{-1})
$1_{1,0} \rightarrow 1_{1,1}$	1.19 x 10^{-12}	$1_{0,1} \rightarrow 0_{0,0}$	5.31 x 10^{-7}
$2_{1,2} \rightarrow 1_{1,1}$	3.76 x 10^{-6}	$2_{1,1} \rightarrow 1_{1,0}$	3.89 x 10^{-6}
$2_{1,1} \rightarrow 2_{1,2}$	1.08 x 10^{-11}	$2_{0,2} \rightarrow 1_{0,1}$	5.10 x 10^{-6}
$3_{1,3} \rightarrow 2_{1,2}$	1.61 x 10^{-5}	$3_{1,2} \rightarrow 2_{1,1}$	1.67 x 10^{-5}
$3_{1,2} \rightarrow 3_{1,3}$	4.30 x 10^{-11}	$3_{0,3} \rightarrow 2_{0,2}$	1.84 x 10^{-5}
$4_{1,4} \rightarrow 3_{1,3}$	4.18 x 10^{-5}	$4_{1,3} \rightarrow 3_{1,2}$	4.32 x 10^{-5}
$4_{1,3} \rightarrow 4_{1,4}$	1.19 x 10^{-10}	$4_{0,4} \rightarrow 3_{0,3}$	4.53 x 10^{-5}
$5_{1,5} \rightarrow 4_{1,4}$	8.54 x 10^{-5}	$5_{1,4} \rightarrow 4_{1,3}$	8.84 x 10^{-5}
$5_{1,4} \rightarrow 5_{1,5}$	2.69 x 10^{-10}	$5_{0,5} \rightarrow 4_{0,4}$	9.05 x 10^{-5}
$6_{1,6} \rightarrow 5_{1,5}$	1.52 x 10^{-4}	$6_{1,5} \rightarrow 5_{1,4}$	1.57 x 10^{-4}
$6_{1,5} \rightarrow 6_{1,6}$	5.27 x 10^{-10}	$6_{0,6} \rightarrow 5_{0,5}$	1.59 x 10^{-4}
$7_{0,7} \rightarrow 6_{0,6}$	2.55 x 10^{-4}	$8_{0,8} \rightarrow 7_{0,7}$	2.36 x 10^{-4}
$9_{0,9} \rightarrow 8_{0,8}$	5.21 x 10^{-4}		

Table 2 - Einstein A-coefficients for *b*-type transitions

Transition	A-coefficient (s^{-1})	Transition	A-coefficient (s^{-1})
$1_{1,0} \rightarrow 1_{0,1}$	5.45 x 10^{-5}	$1_{1,1} \rightarrow 0_{0,0}$	4.11 x 10^{-5}
$1_{1,1} \rightarrow 2_{0,2}$	1.40 x 10^{-5}	$2_{1,2} \rightarrow 1_{0,1}$	4.15 x 10^{-5}
$2_{1,2} \rightarrow 3_{0,3}$	1.46 x 10^{-5}	$2_{1,1} \rightarrow 2_{0,2}$	5.46 x 10^{-5}
$3_{1,2} \rightarrow 3_{0,3}$	5.47 x 10^{-5}	$3_{1,3} \rightarrow 2_{0,2}$	4.42 x 10^{-5}
$3_{1,3} \rightarrow 4_{0,4}$	1.34 x 10^{-5}	$4_{1,4} \rightarrow 3_{0,3}$	4.79 x 10^{-5}
$4_{1,4} \rightarrow 5_{0,5}$	1.19 x 10^{-5}	$4_{1,3} \rightarrow 4_{0,4}$	5.48 x 10^{-5}
$5_{1,4} \rightarrow 5_{0,5}$	5.50 x 10^{-5}	$5_{1,5} \rightarrow 4_{0,4}$	5.21 x 10^{-5}
$5_{1,5} \rightarrow 6_{0,6}$	1.03 x 10^{-5}	$6_{1,6} \rightarrow 5_{0,5}$	5.68 x 10^{-5}
$6_{1,6} \rightarrow 7_{0,7}$	8.75 x 10^{-6}	$6_{1,5} \rightarrow 6_{0,6}$	5.52 x 10^{-5}

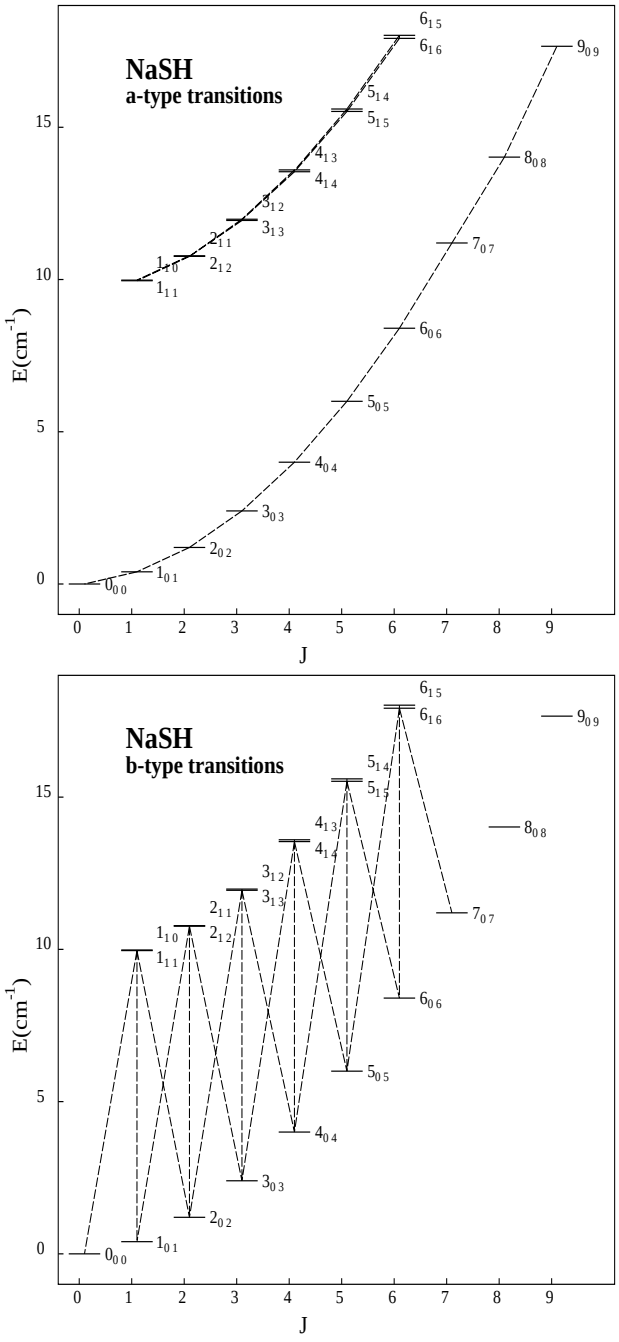

Fig. 1 - Rotational energy levels in the ground vibrational state of NaSH along with radiative transitions