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Einstein A - Coefficient of Isomer 3 of C_5H_2 Molecule

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ABSTRACT

Laboratory formation of four isomers of C_5H_2 molecule is reported. For identification of a molecule in cosmic objects, one of the required input data is Einstein A- coefficients (radiative transition probabilities) for the molecule. Here, we report Einstein A- coefficients for electric dipole transitions in the isomer 2 of C_5H_2 among the rotational levels of the ground electronic and ground vibrational states up to 21 cm^{-1}.

Keywords: C_5H_2 molecule, isomers, molecular data.

I. INTRODUCTION

More than 150 molecules detected in cosmic object, most of them are hydrogen-carbon compounds. After detection of C3H2, both linear as well as cyclic isomers in the cosmic objects, astronomers showed interest in the search of C_5H_2molecule.

The isomer 3 of C_5H_2 (Penta-tetra-enylidine) molecule has been observed in laboratory by Gottlieb *et al.*(1998) . It is an asymmetric top planar molecule having an electric dipole moment μ = 4.8 Debye which is inclined with theaxes of inertia. So that its components along the a and b axes of inertia are μ_a= 2.84 Debye and μ_b = 3.86 Debye. Thus, this isomer like isomer1 has both the a and b type radiative transitions and therefore the rotational energy levels cannot be separated into two different groups, as is done in case of isomer 2. For this isomer only a type transitions have been observed and given in Table 2. The molecular and distortional data derived by Gottlieb *et al.* 1998. For this isomer of C_5H_2 are given in Table 1.

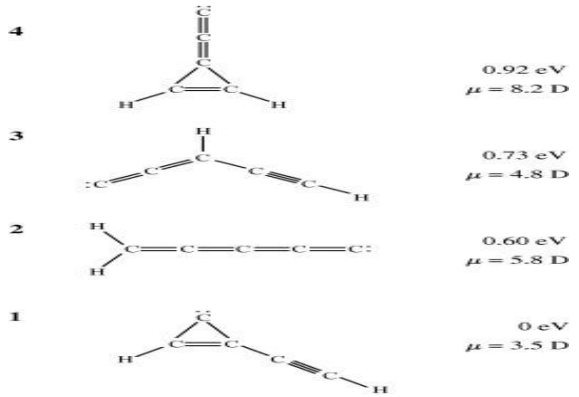

Fig. 1. Structure of four isomers of C_5H_2molecule along with electric dipole moment and their energy

Table 1: Molecular data of isomer 3 of C_5H_2 molecule

Constants	Isomer 3
A (MHz)	318166
B (MHz)	2865.77293
C (MHz)	2624.47953
Δ_J (MHz)	$14.718x\ 10^{-4}$
Δ_{JK} (MHz)	$-13.97x10^{-2}$
μ_a (Debye)	2.84
μ_b (Debye)	3.86

Table 2: Measured rotational frequencies of isomer 3 of C_5H_2 molecule.

Transition	Frequency (MHz)
$1_{01} \rightarrow 0_{00}$	5490.247
$2_{12} \rightarrow 1_{11}$	10739.735
$2_{02} \rightarrow 1_{01}$	10978.956
$2_{11} \rightarrow 1_{10}$	11222.297
$3_{13} \rightarrow 2_{12}$	16108.601
$3_{03} \rightarrow 2_{02}$	16464.592
$3_{12} \rightarrow 2_{11}$	16832.396
$4_{14} \rightarrow 3_{13}$	21476.273
$4_{04} \rightarrow 3_{12}$	21945.622
$4_{13} \rightarrow 3_{12}$	22441.222

II. CALCULATIONS

For calculation of the Einstein A-coefficients, the required input data are the molecular rotational and distortional constants and the electric dipole moment are reported in Table 1. Details for calculations of Einstein A-coefficients for a-type rotational transitions in an asymmetric top molecule are discussed by Chandra and Sharma(1994) , Chandra and Rashmi (1998) .By using the data given in Table 1, values for a-type rotational transitions in the ground electronic and ground vibrational states of the isomer 3 of C_5H_2 among the levels up to 21 cm-1 are computed, and are given in Tables 3 and 4.

III. RESULT

The Einstein A-coefficients can be used for computing mean radiative lifetimes of the energy levels(Chandra, 2002) . One can easily find out that some pairs of successive levels connected by radiative transitions show that the mean radiative lifetime of the upper level is larger than that of the lower one.

Table 3: Einstein A-coefficients for a-type ortho transitions in isomer 3 of C_5H_2.

Transitions	A- coeff. (s-1)	Transitions	A- coeff. (s-1)
$1_{10} \rightarrow 1_{11}$	6.61×10^{-13}	$2_{12} \rightarrow 1_{11}$	3.50×10^{-8}
$2_{11} \rightarrow 1_{10}$	3.99×10^{-5}	$2_{11} \rightarrow 2_{12}$	5.95×10^{-10}
$3_{13} \rightarrow 2_{12}$	1.50×10^{-7}	$3_{12} \rightarrow 2_{11}$	1.71×10^{-7}
$3_{12} \rightarrow 3_{13}$	2.38×10^{-11}	$4_{14} \rightarrow 3_{13}$	3.88×10^{-7}
$4_{13} \rightarrow 3_{12}$	4.43×10^{-7}	$5_{15} \rightarrow 4_{14}$	7.94×10^{-7}
$5_{14} \rightarrow 4_{13}$	9.06×10^{-7}	$5_{14} \rightarrow 5_{15}$	1.49×10^{-10}
$6_{16} \rightarrow 5_{15}$	1.41×10^{-6}	$6_{15} \rightarrow 5_{14}$	1.61×10^{-6}
$6_{15} \rightarrow 6_{16}$	2.92×10^{-10}	$7_{17} \rightarrow 6_{16}$	2.28×10^{-6}
$7_{16} \rightarrow 6_{15}$	2.60×10^{-6}	$7_{16} \rightarrow 7_{17}$	5.18×10^{-10}
$8_{18} \rightarrow 7_{17}$	3.45×10^{-6}	$8_{17} \rightarrow 7_{16}$	3.93×10^{-6}
$8_{17} \rightarrow 8_{18}$	8.57×10^{-10}	$9_{19} \rightarrow 8_{18}$	4.96×10^{-6}
$9_{18} \rightarrow 8_{17}$	5.65×10^{-6}	$9_{18} \rightarrow 9_{19}$	1.34×10^{-9}
$3_{31} \rightarrow 1_{12}$	2.23×10^{-9}	$3_{31} \rightarrow 3_{12}$	1.60×10^{-9}

Table 4: Einstein A-coefficients for a-type para transitions in isomer 3 of C_5H_2

Transitions	A- coeff. (s-1)	Transitions	A- coeff. (s-1)
$1_{01} \rightarrow 0_{00}$	5.29×10^{-9}	$2_{02} \rightarrow 1_{01}$	4.98×10^{-8}
$3_{03} \rightarrow 2_{02}$	1.80×10^{-7}	$4_{04} \rightarrow 3_{03}$	4.42×10^{-7}
$5_{05} \rightarrow 4_{04}$	8.82×10^{-7}	$6_{06} \rightarrow 5_{05}$	1.54×10^{-6}
$2_{21} \rightarrow 2_{02}$	1.27×10^{-9}	$2_{20} \rightarrow 1_{01}$	1.00×10^{-9}
$2_{20} \rightarrow 3_{03}$	3.22×10^{-10}	$3_{22} \rightarrow 3_{03}$	3.19×10^{-9}
$3_{22} \rightarrow 2_{21}$	1.00×10^{-7}	$3_{21} \rightarrow 2_{02}$	2.71×10^{-9}
$3_{21} \rightarrow 4_{04}$	7.29×10^{-10}	$3_{21} \rightarrow 2_{20}$	1.00×10^{-9}
$7_{07} \rightarrow 6_{06}$	2.48×10^{-6}	$4_{23} \rightarrow 4_{04}$	5.74×10^{-9}
$4_{23} \rightarrow 3_{22}$	3.22×10^{-7}	$4_{22} \rightarrow 3_{03}$	5.35×10^{-9}
$4_{22} \rightarrow 5_{05}$	1.14×10^{-9}	$4_{22} \rightarrow 3_{21}$	3.33×10^{-7}
$8_{08} \rightarrow 7_{07}$	3.71×10^{-6}	$5_{24} \rightarrow 5_{05}$	8.92×10^{-9}
$5_{24} \rightarrow 4_{23}$	7.43×10^{-7}	$5_{23} \rightarrow 4_{04}$	9.19×10^{-9}
$5_{23} \rightarrow 6_{06}$	1.49×10^{-9}	$5_{23} \rightarrow 4_{22}$	7.46×10^{-7}

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