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Einstein A- Coefficient of Isomer 2 of C_5H_2Molecule

Shinde S. A.

Department of Physics, Sharadchandra A C S college Naigaon(Bz.) Dist- Nanded (M.S.) India

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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 upto 21 cm^{-1}.

Keywords: C_5H_2 molecule, molecular data.

INTRODUCTION

The isomer 2 of C_5H_2 (Pentatetraenylidine) molecule has been observed in laboratory by Travers *et.al*[1]. and McCarthy *et.al.*[2]This isomer is an a type asymmetric top planar molecule having a large electric dipole moment μ = 5.8 Debye along the a- axis of inertia. The molecular and distortional data derived by Travers *et al.*[1] and McCarthy *et.al.*[2] for this isomer of C_5H_2 are given in **Table 1**. Measured a- type transitions for the isomer 2 are given in **Table 2**.

Table 1: Molecular data of isomer 2 of C_5H_2 molecule

Constants	Isomer 2
A (MHz)	277,600
B (MHz)	2304.78443
C (MHz)	2285.80533
Δ_J (MHz)	1.046×10^{-4}
Δ_{JK} (MHz)	4.642×10^{-2}
μ_a (Debye)	5.8

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

Transition	Frequency (MHz)
$3_{13} \rightarrow 2_{12}$	13743.013
$3_{03} \rightarrow 2_{02}$	13771.755
$3_{12} \rightarrow 2_{11}$	13799.945
$4_{14} \rightarrow 3_{13}$	18324.000
$4_{04} \rightarrow 3_{03}$	18362.323
$4_{13} \rightarrow 3_{12}$	18399.918
$5_{15} \rightarrow 4_{14}$	22904.980
$5_{05} \rightarrow 4_{04}$	22952.877
$5_{14} \rightarrow 4_{13}$	22999.878

MATERIAL AND METHODS

For calculation of the Einstein A-coefficients, the required input data are the molecular rotational and distrotional 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[3], Chandra and Rashmi[4].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 2 of C_5H_2 among the levels up to 21 cm^{-1} are computed, and are given in **Tables 3 and 4**.

RESULT

Table 3: Einstein A-coefficients for a-type ortho transitions in isomer 2 of C_5H_2

Transitions	A- coeff. (s^{-1})	Transitions	A- coeff. (s^{-1})
$2_{12} \rightarrow 1_{11}$	9.03×10^{-8}	$2_{11} \rightarrow 1_{10}$	9.15×10^{-8}
$3_{13} \rightarrow 2_{12}$	3.83×10^{-7}	$3_{12} \rightarrow 2_{11}$	3.92×10^{-7}
$4_{14} \rightarrow 3_{13}$	1.00×10^{-6}	$4_{13} \rightarrow 3_{12}$	1.02×10^{-6}
$4_{13} \rightarrow 4_{14}$	1.34×10^{-13}	$5_{15} \rightarrow 4_{14}$	2.05×10^{-6}
$5_{14} \rightarrow 4_{13}$	2.08×10^{6}	$5_{14} \rightarrow 4_{15}$	3.01×10^{-13}
$6_{16} \rightarrow 5_{15}$	3.65×10^{-6}	$6_{15} \rightarrow 5_{14}$	3.69×10^{-6}
$6_{15} \rightarrow 6_{16}$	5.90×10^{-13}	$7_{17} \rightarrow 6_{16}$	5.90×10^{-6}
$7_{16} \rightarrow 6_{15}$	5.98×10^{-6}	$7_{16} \rightarrow 7_{17}$	1.05×10^{-12}
$8_{18} \rightarrow 7_{17}$	8.93×10^{-6}	$8_{17} \rightarrow 7_{16}$	9.04×10^{-6}
$8_{17} \rightarrow 8_{18}$	1.73×10^{-12}	$9_{19} \rightarrow 8_{18}$	3.83×10^{-11}
$9_{18} \rightarrow 8_{17}$	5.51×10^{-11}	$9_{18} \rightarrow 9_{19}$	2.20×10^{-10}
$10_{1,10} \rightarrow 9_{19}$	3.39×10^{-6}	$10_{9,19} \rightarrow 9_{18}$	3.43×10^{-6}
$10_{19} \rightarrow 10_{1,10}$	3.28× 10-10	$11_{1,10} \rightarrow 11_{1,11}$	7.05×10^{-10}

The Einstein A-coefficients can be used for computing mean radiative lifetimes of the energy levels[5]. 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 4: Einstein A-coefficients for a-type para transitions in isomer 2 of C_5H_2

Transitions	A- coeff. (s^{-1})	Transitions	A- coeff. (s^{-1})
$1_{01} \rightarrow 0_{00}$	1.26×10^{-8}	$2_{02} \rightarrow 1_{01}$	1.21×10^{-7}
$3_{03} \rightarrow 2_{02}$	4.38×10^{-7}	$4_{04} \rightarrow 3_{03}$	1.08×10^{-6}
$5_{05} \rightarrow 4_{04}$	2.15×10^{-6}	$6_{06} \rightarrow 5_{05}$	3.78×10^{-6}
$7_{07} \rightarrow 6_{06}$	6.06×10^{-6}	$8_{08} \rightarrow 7_{07}$	1.76×10^{-10}
$9_{09} \rightarrow 8_{08}$	2.73×10^{-6}	$11_{0,11} \rightarrow 10_{0,10}$	4.16×10^{-6}

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*** Corresponding author: Shinde S. A.;**

Department of Physics, Sharadchandra A C S college Naigaon(Bz.)
Dist- Nanded (M.S.) India