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Spectroscopic constants and potential energy curve of the iodine weakly bound 1_u state correlating with the $I(^2P_{1/2}) + I(^2P_{1/2})$ dissociation limit

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Abstract

The stepwise three-step three-color laser population of the $I_2(\beta 1_g, \nu_\beta, J_\beta)$ rovibronic states via the $B0_u^+$, ν_B, J_B rovibronic states and rovibronic levels of the $1_u(bb)$ and $0_g^+(bb)$ states mixed by hyperfine interaction is used for determination of rovibronic level energies of the weakly bound $I_2(1_u(bb))$ state. Dunham coefficients of the state, Y_{i0} ($i = 0$–3), Y_{i1} ($i = 0$–2), Y_{02} and Y_{12} for the $v_{1_u} = 1$–5, 8, 10, 15 and $J_{1_u} \approx 9$–87 ranges, the dissociation energy of the state, D_e, and equilibrium I–I distance, R_e, as well as the potential energy curve are determined. There are aperiodicities in the excitation spectrum corresponding to the β, $\nu_\beta = 23$, $J_\beta \leftarrow 1_u(bb)$, $\nu_{1u} = 4$, 5, J_{1u} progressions in the $I_2 + Rg = He$, Ar mixture, namely, a great number of lines which do not coincide with the R or P line progressions. Their positions conflict with the ΔJ-even selection rule. Furthermore, they do not correspond to the ΔJ-odd progression.

Keywords: iodine molecule, weakly-bound states, dunham coefficients, potential energy curve

(Some figures may appear in colour only in the online journal)

1. Introduction

Among 23 valence states of iodine molecules [1], only deeply bound $X0_g^+(aa)$, $A'2_u(aa)$, $A1_u(aa)$ and $B0_u^+(ab)$ states correlating with the $I(^2P_{3/2}) + I(^2P_{3/2})$ (aa) and $I(^2P_{3/2}) + I(^2P_{1/2})$ (ab) are well studied experimentally [2–15]. For weakly bound $B'0_u^-(aa)$, $a1_g(aa)$, $B''1_u(aa)$, $a'0_g^+(aa)$, $c1_g(ab)$, $0_g^+(ab)$, $0_g^-(ab)$ and $b'(ab)$ states, only some spectroscopic characteristics are known [2–4, 16–18].

In 2007, T Ridley *et al* [19, 20] measured rotationally unresolved $I_2(D0_u^+, F0_u^+ \rightarrow 0_g^+(bb))$ and $I_2(1_g(^1D_2)) \rightarrow 1_u(bb))$ luminescence spectra. They simulated these spectra and obtained some spectroscopic parameters (T_e, D_e, ω_e, B_e and R_e) of the lower states. Uncertainties of these parameters are rather high, $\pm 2\ cm^{-1}$ for T_e and D_e, and $\pm 0.2\ cm^{-1}$ for ω_e.

Recently [21], we reported on results of determination of the rovibronic level energies of the $0_g^+(bb)$ state that were more precise than in [19, 20]. The Dunham parameters of the state, Y_{i0} ($i = 0$–3), Y_{i1} ($i = 0$–3) and Y_{02} for the $v_{0_g^+} = 0$–16 and $J_{0_g^+} \approx 14$–135 ranges, as well as R_e and D_e values were determined. The potential energy curve (PEC) of the state was also given.

Very recently, we have estimated upper limit of electric dipole forbidden $I_2(1_u(bb) \leftarrow B0_u^+)$ transition cross section. We have shown that the integral cross-section of the transition at fundamental harmonics of a Nd:YAG laser, $\nu_f^1 = 9395.12\ cm^{-1}$, $\nu_f^2 = 9393.53\ cm^{-1}$ and $\nu_f^3 = 9396.67\ cm^{-1}$, $\Sigma = \int \sigma(\nu) d\nu$, is low and does not exceed 1.7×10^{-19} cm, so the effective cross section $\sigma_{1u-B}^{eff} \leqslant \Sigma/\Delta\nu \approx 4 \times 10^{-18}\ cm^2$ ($\Delta\nu \approx 0.04\ cm^{-1}$) [22]. We have also shown that rovibronic levels of three $0_{g,}^+0_{u,}^-1_u(bb)$ states are mixed by hyperfine interaction. The $I_2(1_u(bb) \leftarrow B0_u^+)$ transition is allowed due to hyperfine mixing of the $1_u(bb)$, ν_{1u}, $J_{1u}/0_g^+(bb)$, ν_0, J_0 rovibronic states [23].

