IOP Publishing Journal of Physics B: Atomic, Molecular and Optical Physics
J. Phys. B: At. Mol. Opt. Phys. **48** (2015) 055101 (8pp) doi:10.1088/0953-4075/48/5/055101

# Spectroscopic constants and potential energy curves of some iodine valence ungerade weakly bound states

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Received 13 November 2014, revised 30 December 2014
Accepted for publication 13 January 2015
Published 11 February 2015

**Abstract**

Luminescence spectra corresponding to transitions from $\beta 1_g$, $G1_g$, $D'2_g$, and $g0_g^-$ ion-pair states of an iodine molecule to weakly bound valence states $1_u$, $2_u$, and $0_u^-$, correlating with the $I(^2P_{3/2})+I(^2P_{1/2})$ $(ab)$ and $I(^2P_{1/2})+I(^2P_{1/2})$ $(bb)$ dissociation limits, respectively, have been observed and analyzed. Energies of vibrational levels, spectroscopic constants, and potential energy curves of the valence states have been determined. The $0_u^-$ state is shown to be bound by 488(2) $cm^{-1}$ and placed lower than $1_u(bb)$ and $0_g^+(bb)$, unlike *ab initio* estimations.

S Online supplementary data available from stacks.iop.org/JPB/48/055101/mmedia

Keywords: diatomic molecules, valence states, weakly bound states, hyperfine coupling

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

## 1. Introduction

The iodine molecule has 23 valence states that are grouped by correlation with three dissociation limits: $I(^2P_{3/2})+I(^2P_{3/2})$ $(aa)$, $I(^2P_{3/2})+I(^2P_{1/2})$ $(ab)$, and $I(^2P_{1/2})+I(^2P_{1/2})$ $(bb)$. Though valence states of $I_2$ have been widely investigated (see [1–17] and references therein), only four deeply bound (dissociation energy exceeds 1000 $cm^{-1}$) states are well described: $X0_g^+(aa)$, $A'2_u(aa)$, $A1_u(aa)$, and $B0_u^+(ab)$. Spectroscopic constants and potential energy curves (PECs) of these states have been determined with high precision from analysis of experimental data [4–10]. The remaining nineteen states are weakly bound and characterized less precisely or not defined at all in some cases. Some spectroscopic characteristics of 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 $b'2_u(ab)$ states are presented in [1–3, 15–18].

Most of the spectroscopic characteristics of the weakly bound valence states have been determined from analysis of luminescence in transitions from the ion-pair (IP) to valence states (see [7, 15–17, 19–21] and references). For example, optical transitions to the $2_g(aa)$, $0_u^-(ab)$, $1_g(ab)$, $1_u(ab)$, and $2_g(ab)$ states from the IP states were observed and used for the determination of their PECs (see [19–21] and references).

Until recently, there were only two works on experimental analysis of three $0_g^+$, $1_u$, and $0_u^-$ states correlating with the third, $bb$, dissociation limit, both published by Ridley *et al* [20, 21]. Vibrationally resolved emission spectra from $D0_u^+$, $F0_u^+$, and $1_g(^1D_2)$ IP states rovibronic levels to the $0_g^+(bb)$ and $1_u(bb)$ states were measured and successfully simulated, and some spectroscopic parameters ($T_e$, $D_e$, $\omega_e$, $B_e$, and $R_e$) of $0_g^+(bb)$ and $1_u(bb)$ states were obtained. Very recently, we also reported [22, 23] on Dunham coefficients ($Y_{ij}$) of these $(bb)$ states determined with higher accuracy as result of analysis of the $D0_u^+ \leftarrow 0_g^+(bb)$ and $\beta 1_g \leftarrow 1_u(bb)$ transitions. The $D0_u^+$ and $\beta 1_g$ states were populated using a three-step three-color $IP \leftarrow (bb) \leftarrow B0_u^+ \leftarrow X0_g^+$ laser excitation scheme in these studies. Rotational as well as rovibrational energy transfer processes in the $(bb)$ states induced by collisions with He and Ar atoms were used for population of a wide range of rovibronic levels. In such a way, we were able to observe more than 300 transitions in spectra and successfully determined molecular parameters of the lower valence states. As to the $0_u^-(bb)$ state, no experimental

 